

## Supporting Information

### Comparing the Oxygen Reduction Reaction on Selectively Edge Halogen Doped Graphene from Quantum Mechanics

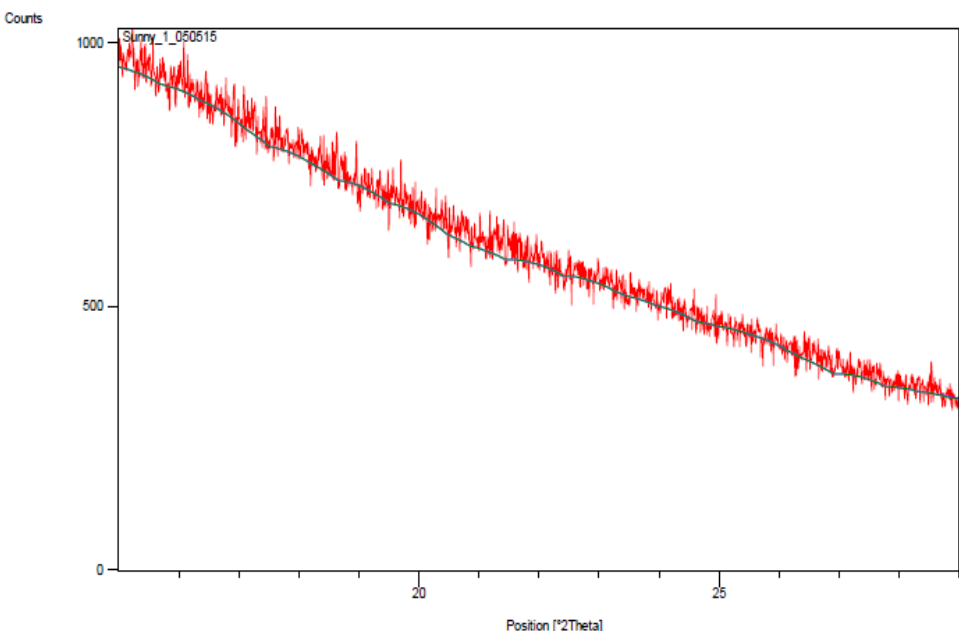
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#### Synthesis of Graphene Iodide

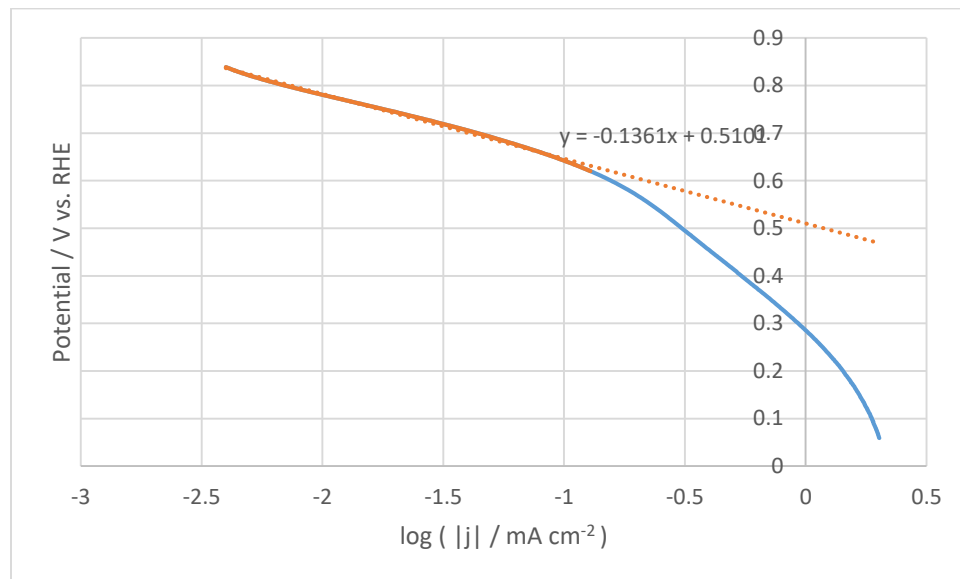
5g graphite and 2g iodine were put into a planetary ball mill for 168 hrs at 1500 rpm with stainless steel balls. The resultant product was extracted with methanol to remove organic impurity and excess iodine, followed by extraction with 1M HCl solution to remove metal impurities. Product was freeze dried at 78.5°C at reduced pressure for 48 hrs. The final graphene product did not contain any graphite peak (26.5°) according to the X-ray diffraction pattern in Figure S1.



**Figure S1.** X-ray diffraction pattern of synthesized graphene halide. Graphite peak (26.5°) disappeared due to the synthesis reaction.

## Linear Sweep Voltammograms (LSV) of Graphene Halide

The graphene electrocatalyst suspension is created by mixing 18.5 mg of graphene iodide with a pre-prepared 25 mL 24% isopropyl solution, followed by addition of 100 mL of Nafion solution. The solution is then sonicated for 30 minutes. 10  $\mu\text{L}$  of the suspension is dried on the glassy carbon rotating disk electrode (RDE) tip for one hour. The LSV measurements on the RDE was carried out in  $\text{O}_2$ -saturated 0.1 M KOH at a scan rate of 0.01 V/s at 1600 rpm. The reference electrode was Ag/AgCl. Figure S2 shows the plot of the  $\log(\text{mA cm}^{-2})$  vs. potential. The potential is converted from the Ag/AgCl reference electrode to the reversible hydrogen electrode (RHE) by the equation  $V(\text{RHE}) = V(\text{Ag/AgCl}) + 0.0593(\text{pH}_{\text{Ag/AgCl}} - \text{pH}_{\text{RHE}}) + 0.288$ .



**Figure S2.**  $\log ( |j| )$  vs. potential. The Tafel slope of the onset potential region for graphene iodide is determined to be 0.136 V/dec.

## ER Mechanism – ZU Chlorine

### 1) OOH formation

#### a. Initial

C	2.16038739	1.17533764	-0.19832923
C	4.27981670	-0.04061895	-0.07154026
C	6.41045470	-1.27511864	-0.08582450
C	8.54381943	-2.51751503	-0.09371919
C	10.67563631	-3.76436480	-0.06752309
C	4.29313040	2.39847928	0.17553268
C	6.40771902	1.19206539	-0.07533457
C	9.96077052	-0.04893433	-0.08627511
C	10.67240686	-1.28688911	-0.06943327

C	12.77806427	-2.53288311	0.01718780
C	6.42105897	3.63771727	-0.19560298
C	8.54170953	2.42061969	-0.07184805
C	10.67208406	1.18078716	-0.08652712
C	12.80681259	-0.06257627	-0.10618741
C	14.95335393	-1.27591033	0.02500328
C	8.55666934	4.85831868	0.17369439
C	10.67120721	3.64911193	-0.07809627
C	12.80480478	2.41256939	-0.10234481
C	14.93805933	1.17517264	-0.06755912
C	17.07670067	-0.06965073	-0.06507248
C	3.56271986	1.20530477	-0.02951376
C	5.69814506	-0.03779143	-0.06688957
C	7.83117939	-1.27839325	-0.09972613
C	9.96200670	-2.51780650	-0.06500130
C	12.08546866	-3.72137694	0.13224434
C	5.68965917	2.43840788	-0.03492640
C	7.82684461	1.19439768	-0.10309768
C	12.08689948	-1.29408236	-0.08339323
C	14.25080717	-2.57326756	-0.07724600
C	7.82452982	3.66651140	-0.02984604
C	9.96049681	2.41941046	-0.06880532
C	12.09721093	1.17285381	-0.09940654
C	14.23232761	-0.05354028	-0.08191560
C	16.33138399	-1.26678824	0.14272128
C	9.95351638	4.89520351	-0.03816272
C	12.09097548	3.65152716	-0.10576279
C	14.22497685	2.41230241	-0.08608981
C	16.35817900	1.17339581	-0.06344965
C	18.46934209	-0.03250801	-0.29330177
Cl	17.13365905	-2.72600700	0.63980235
Cl	14.64636460	-3.24255966	-1.80059874
Cl	12.95266512	-5.14722537	0.61416558

Cl	7.79014445	6.19361016	0.97119287
Cl	5.63242977	5.00633903	-0.91443016
Cl	3.52239472	3.73258962	0.97155011
Cl	1.37275320	2.54116943	-0.92276057
Cl	19.22547950	-1.35032885	-1.12890227
C	8.53932434	-0.04408610	-0.10115849
O	16.15820471	0.20844418	3.28684367
O	15.77808375	-0.42466671	4.29122583
H	14.08491285	-1.46097700	3.60449354
O	13.32075153	-1.83050239	3.13148871
H	12.59968673	-1.79175367	3.77839446
H	14.67897811	-3.32121866	0.59484416

**b. Transition State 1**

C	2.21239511	1.19922786	-0.20846096
C	4.33539061	-0.01670905	-0.07458884
C	6.46759823	-1.25648422	-0.07103041
C	8.60059046	-2.49846318	-0.12186292
C	10.72983057	-3.74561158	-0.27097455
C	4.34908435	2.42441022	0.15823295
C	6.46694780	1.21322134	-0.07430358
C	10.01974202	-0.03093270	-0.08142469
C	10.73320102	-1.27384645	-0.10051551
C	12.86637145	-2.51236292	-0.27004099
C	6.47699182	3.66205936	-0.20416201
C	8.59709602	2.44249604	-0.07245062
C	10.73004495	1.20371542	-0.07627262
C	12.86554168	-0.03513262	-0.12488136
C	14.99564965	-1.28447528	-0.20443809
C	8.61307809	4.88156490	0.17334566
C	10.72829689	3.67287334	-0.07399421
C	12.85964792	2.43567826	-0.09047201
C	14.99456856	1.18882856	-0.06961463
C	17.12826110	-0.05283648	-0.20529887

C	3.61604983	1.23143257	-0.04655825
C	5.75447721	-0.01562099	-0.05989059
C	7.88857295	-1.25865477	-0.08996023
C	10.01834941	-2.50145979	-0.15713333
C	12.13771985	-3.72199137	-0.16781505
C	5.74830988	2.46104976	-0.04252356
C	7.88487199	1.21427986	-0.09907907
C	12.15270155	-1.26512454	-0.15942257
C	14.26777928	-2.46017447	-0.48972251
C	7.87881066	3.69026965	-0.03752863
C	10.01633585	2.44356510	-0.05975897
C	12.15102852	1.20241947	-0.09324412
C	14.28199117	-0.03878967	-0.11701350
C	16.40035723	-1.25642494	-0.04809561
C	10.01008459	4.91910342	-0.03878062
C	12.14557744	3.67530091	-0.09875931
C	14.28065110	2.42951929	-0.07071010
C	16.41346695	1.19318649	-0.11418873
C	18.51038586	-0.01214548	-0.48219522
Cl	17.20486616	-2.65508479	0.57626216
Cl	15.03333960	-3.72821282	-1.38827438
Cl	12.95921407	-5.13405097	0.41803830
Cl	7.85104054	6.20585103	0.99595350
Cl	5.69446731	5.03900957	-0.91121484
Cl	3.57638807	3.76153703	0.95002790
Cl	1.41349608	2.56570517	-0.91825651
Cl	19.22831910	-1.31385056	-1.37241475
C	8.59852604	-0.02627027	-0.09223597
O	16.23428070	-0.31537180	2.60713921
O	15.39781319	-0.79916940	3.55376130
H	14.83607165	-1.51045157	3.11660677
O	13.14067724	-2.33493081	3.02967278
H	12.39283389	-1.88127601	3.44397335

H 12.90062742 -2.38410717 2.08523665

**c. Transition State 2**

C	2.22206465	1.22226959	-0.19020335
C	4.34904751	0.01529554	-0.07731312
C	6.48161413	-1.22409443	-0.07933628
C	8.61524144	-2.46567166	-0.17974758
C	10.74948572	-3.71415636	-0.37427069
C	4.36250764	2.45560031	0.14279566
C	6.48027893	1.24475375	-0.07960563
C	10.03376941	0.00226624	-0.11975356
C	10.74636153	-1.23739918	-0.19429830
C	12.88742384	-2.48142559	-0.35936495
C	6.50390877	3.69561702	-0.18682130
C	8.61491108	2.47057560	-0.06083730
C	10.74571088	1.23291935	-0.09482922
C	12.88133799	-0.00515692	-0.17719837
C	15.01755602	-1.25031631	-0.24964031
C	8.63726461	4.89963657	0.24094144
C	10.74593167	3.69742077	-0.06263781
C	12.87690759	2.46502480	-0.09423722
C	15.01192042	1.22046238	-0.07635821
C	17.14375708	-0.02004668	-0.23389425
C	3.62914254	1.26306930	-0.05107101
C	5.76764783	0.01623391	-0.06695771
C	7.90243167	-1.22682471	-0.11702177
C	10.03414707	-2.46623402	-0.25595865
C	12.15956596	-3.69376853	-0.27837716
C	5.76307225	2.49445602	-0.04973581
C	7.90014757	1.24523389	-0.10011465
C	12.16793984	-1.23466361	-0.24458524
C	14.29309824	-2.42933044	-0.53658605
C	7.90011077	3.71709003	-0.00270539
C	10.03314510	2.46978366	-0.05941032

C	12.16714478	1.23241155	-0.11717218
C	14.30030521	-0.00748727	-0.14297296
C	16.42152178	-1.22771311	-0.09617977
C	10.02931590	4.94181457	-0.00572570
C	12.16321459	3.70466151	-0.09756525
C	14.29802070	2.46137476	-0.07344655
C	16.43011188	1.22531243	-0.13647853
C	18.52075003	0.01619780	-0.54119437
Cl	17.23040230	-2.62977915	0.52724084
Cl	15.07650690	-3.68556182	-1.44073267
Cl	12.97508241	-5.11361500	0.29443740
Cl	7.90140720	6.17967209	1.15005069
Cl	5.74664184	5.10196445	-0.86292306
Cl	3.59005719	3.79723955	0.92424486
Cl	1.38458117	2.58208323	-0.86639336
Cl	19.20566580	-1.29054912	-1.45339438
C	8.61324075	0.00532168	-0.10943344
O	16.29479979	-0.46076620	2.64566227
O	15.19311649	-1.24421108	2.65585797
H	15.48750509	-2.09319830	3.06454261
O	12.73468727	-2.42110690	3.19847661
H	11.93860030	-1.95588998	3.48576860
H	12.81637094	-2.18864315	2.25889145

**d. Transition State 3**

C	2.21509435	1.22638263	-0.21128636
C	4.33903519	0.01800984	-0.06996188
C	6.47345098	-1.21878014	-0.07933398
C	8.60842222	-2.45757474	-0.18474789
C	10.73948782	-3.70560108	-0.38627630
C	4.35247071	2.45451942	0.14959074
C	6.47054747	1.24665534	-0.07668491
C	10.02547121	0.00957844	-0.13155563
C	10.73942858	-1.22918489	-0.21073997

C	12.88445105	-2.47121513	-0.36638348
C	6.48218670	3.69213449	-0.21888865
C	8.60135386	2.47677517	-0.06709685
C	10.73621944	1.24019924	-0.10017921
C	12.87454514	0.00171843	-0.17636602
C	15.01529419	-1.24396573	-0.20046055
C	8.61630569	4.90970093	0.18343382
C	10.73328418	3.70399439	-0.06333893
C	12.86621366	2.47133882	-0.09177411
C	15.00310013	1.23134463	-0.05867451
C	17.13743776	-0.01223535	-0.18809696
C	3.61874908	1.26318140	-0.04664672
C	5.75867517	0.01878207	-0.06217554
C	7.89464283	-1.22037641	-0.12453446
C	10.02718005	-2.45775698	-0.26544169
C	12.15228381	-3.68424673	-0.29501459
C	5.75160039	2.49207615	-0.05157932
C	7.89001890	1.24927613	-0.10212558
C	12.16243967	-1.22704271	-0.25410388
C	14.29517100	-2.42036442	-0.50892301
C	7.88215906	3.72233034	-0.03266070
C	10.02127748	2.47653181	-0.06035479
C	12.15799661	1.23871161	-0.12017926
C	14.29423296	0.00011720	-0.11919685
C	16.41608541	-1.21604249	-0.01026217
C	10.01392609	4.94785287	-0.02587867
C	12.15212356	3.70892317	-0.09385217
C	14.28777992	2.46945924	-0.06849357
C	16.42200603	1.23408576	-0.11835670
C	18.51024367	0.02034042	-0.52271407
Cl	17.23141711	-2.62172389	0.59919320
Cl	15.10993822	-3.67775840	-1.38190048
Cl	12.95974182	-5.10088493	0.29213498



Cl	7.84747738	6.24069772	0.98770208
Cl	5.70387825	5.06161801	-0.94265893
Cl	3.57979020	3.79592857	0.93224770
Cl	1.41813857	2.58368121	-0.93830571
Cl	19.17287309	-1.30407918	-1.42134259
C	8.60401546	0.01120014	-0.11741837
O	16.14205919	-0.52569978	2.46355750
O	15.14559054	-1.43705282	2.64915023
H	15.58687434	-2.18792898	3.10737775
O	12.51931534	-2.52401869	3.18155850
H	11.82088837	-1.91055399	3.44855281
H	12.92883885	-2.09732271	2.40619865

**e. Transition State 4**

C	2.21434669	1.22599835	-0.21241630
C	4.33752918	0.01892023	-0.06956870
C	6.47122006	-1.21507568	-0.07981665
C	8.60583716	-2.45222289	-0.18953724
C	10.72976566	-3.70190277	-0.40089567
C	4.35192638	2.45434066	0.15083330
C	6.46968423	1.24782315	-0.07701995
C	10.02435371	0.00909500	-0.13630186
C	10.73617924	-1.22621856	-0.21596787
C	12.88436618	-2.46097233	-0.38347319
C	6.48136661	3.69212749	-0.21940102
C	8.59974141	2.47790918	-0.06669591
C	10.73385498	1.24247579	-0.10313090
C	12.86888197	0.00597518	-0.18197623
C	15.00909171	-1.23220021	-0.13767900
C	8.61611672	4.90923501	0.18620181
C	10.73121884	3.70480057	-0.06352792
C	12.86255677	2.47400659	-0.09195599
C	14.99644849	1.23936925	-0.03810293
C	17.13125405	-0.00139435	-0.13638048

C	3.61871393	1.26211548	-0.04700140
C	5.75803926	0.01896495	-0.06225289
C	7.89341577	-1.21774132	-0.12881206
C	10.02258555	-2.45577896	-0.26978567
C	12.14841069	-3.67901873	-0.31669305
C	5.75164580	2.49174131	-0.05121120
C	7.88878886	1.24955591	-0.10318107
C	12.16054291	-1.22351235	-0.26062543
C	14.29892409	-2.40372792	-0.49508563
C	7.88175246	3.72145477	-0.03178022
C	10.02012992	2.47672813	-0.05971161
C	12.15449476	1.24082987	-0.12449056
C	14.28874633	0.00534063	-0.09982726
C	16.40351179	-1.18995128	0.16503708
C	10.01344936	4.94690543	-0.02524869
C	12.15051105	3.70928538	-0.09510434
C	14.28479734	2.47234095	-0.06432345
C	16.41852237	1.23929072	-0.09966010
C	18.49586973	0.02417532	-0.51419293
Cl	17.23273102	-2.62818092	0.66761768
Cl	15.13130203	-3.65288895	-1.36397789
Cl	12.95103713	-5.08678271	0.29084155
Cl	7.84885887	6.23791959	0.99370422
Cl	5.70582417	5.06203833	-0.94368679
Cl	3.57993157	3.79331812	0.93678308
Cl	1.41682677	2.58038696	-0.94246902
Cl	19.14115106	-1.31319244	-1.40628275
C	8.60170964	0.01333008	-0.12085224
O	16.11266774	-0.55768197	2.25742515
O	15.12386071	-1.45004370	2.65302073
H	15.62735884	-2.16265758	3.10058671
O	12.47349958	-2.55839829	3.13799590
H	11.82352308	-1.91339486	3.45088454

H	12.97529226	-2.08400217	2.45503700
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**f. Transition State 5**

C	2.21427347	1.22504908	-0.21332543
C	4.33643320	0.02000707	-0.06861961
C	6.47184690	-1.21228158	-0.08092633
C	8.60492290	-2.44832893	-0.19360006
C	10.72276376	-3.69936294	-0.40891556
C	4.35243648	2.45374591	0.15246782
C	6.46994326	1.24811016	-0.07667584
C	10.02435769	0.00781882	-0.13874839
C	10.73366622	-1.22273298	-0.21629003
C	12.88254119	-2.45452355	-0.39265354
C	6.48158112	3.69087399	-0.22056001
C	8.59885017	2.47928990	-0.06607553
C	10.73236222	1.24446662	-0.10448520
C	12.86435853	0.00841410	-0.18808047
C	14.99131246	-1.22583052	-0.12363920
C	8.61666300	4.90879148	0.18704664
C	10.73085793	3.70473305	-0.06357445
C	12.85935432	2.47463802	-0.09291359
C	14.99107885	1.24544064	-0.02535109
C	17.13075906	0.01274319	-0.11785147
C	3.61995335	1.25896907	-0.04681702
C	5.75977069	0.01668916	-0.06151490
C	7.89355038	-1.21656796	-0.13123025
C	10.02067288	-2.45717266	-0.27121235
C	12.14697425	-3.67933926	-0.32426286
C	5.75268710	2.49036930	-0.05103285
C	7.88892861	1.24834558	-0.10412478
C	12.16113384	-1.22349477	-0.26294597
C	14.30135969	-2.39410335	-0.50153138
C	7.88293469	3.71951493	-0.03187706
C	10.02098311	2.47556999	-0.05870623

C	12.15257218	1.24128274	-0.12761511
C	14.28137556	0.00351022	-0.09298837
C	16.37697251	-1.14902713	0.35920947
C	10.01419393	4.94553140	-0.02521324
C	12.15074931	3.70643129	-0.09602364
C	14.28658705	2.46751472	-0.06421053
C	16.42199640	1.24132820	-0.08848122
C	18.48533460	0.02468357	-0.51838596
Cl	17.23667235	-2.64077648	0.68638659
Cl	15.13701072	-3.64697361	-1.35951721
Cl	12.94704070	-5.08137207	0.29531445
Cl	7.84844726	6.23794873	0.99512406
Cl	5.70624842	5.06058071	-0.94653118
Cl	3.58083278	3.79058462	0.93884650
Cl	1.41853929	2.57915605	-0.94471307
Cl	19.13171516	-1.31566219	-1.40427958
C	8.60037253	0.01504274	-0.12254186
O	16.11111632	-0.59062376	2.05769497
O	15.12257909	-1.44555282	2.64758281
H	15.65032373	-2.15022453	3.07950186
O	12.47951414	-2.55763036	3.13918241
H	11.82102173	-1.91965629	3.44981496
H	12.97496407	-2.08547429	2.44909538

**g. Final**

C	2.21501502	1.21893403	-0.22440466
C	4.33636738	0.00741339	-0.06761258
C	6.47079157	-1.22770571	-0.08182975
C	8.60203364	-2.46178500	-0.19590792
C	10.73454484	-3.70550966	-0.42805851
C	4.35043508	2.44344612	0.15861233
C	6.46734495	1.23572579	-0.06996675
C	10.01903437	0.00225013	-0.12836488
C	10.73271482	-1.23571407	-0.22872879

C	12.87355073	-2.46152612	-0.42918988
C	6.47567289	3.68013614	-0.22070546
C	8.59621166	2.46922836	-0.06870256
C	10.72740182	1.23411928	-0.10122905
C	12.86050481	0.00141240	-0.18647878
C	14.97581333	-1.25339084	-0.10554474
C	8.61210034	4.90476835	0.15964163
C	10.72944035	3.69664510	-0.07070564
C	12.86031497	2.46299889	-0.09582012
C	14.99461656	1.22372102	-0.02430901
C	17.15461650	-0.00191081	-0.12547690
C	3.61750500	1.25234631	-0.04590170
C	5.75602688	0.00819832	-0.05809421
C	7.88899576	-1.22592465	-0.13063008
C	10.02290452	-2.46525416	-0.28956006
C	12.15008038	-3.67751768	-0.35345229
C	5.74866771	2.48025614	-0.04204554
C	7.88580186	1.24095547	-0.09792558
C	12.15203759	-1.23002069	-0.28491752
C	14.31141849	-2.39481726	-0.52508890
C	7.87713979	3.71471178	-0.04275243
C	10.01514170	2.47023345	-0.06250071
C	12.14843575	1.23617346	-0.12844276
C	14.26941910	-0.00813620	-0.07244794
C	16.37456756	-1.15960782	0.45972029
C	10.01072758	4.94089009	-0.04319163
C	12.14791237	3.69999380	-0.09595381
C	14.28490252	2.45615641	-0.07226680
C	16.42528919	1.23421176	-0.08387459
C	18.48559505	0.00156142	-0.51409858
Cl	17.22867984	-2.73688903	0.69277024
Cl	15.15422390	-3.63633487	-1.39281945
Cl	12.98383152	-5.09552255	0.19582262

Cl	7.83939784	6.24780995	0.93859294
Cl	5.69013445	5.03874239	-0.95810738
Cl	3.57456519	3.78419812	0.93859384
Cl	1.43101504	2.57655230	-0.96481074
Cl	19.15121705	-1.38041137	-1.32229493
C	8.59923665	0.00466706	-0.11511050
O	16.27185591	-0.63415771	1.83289391
O	15.17340847	-1.27075809	2.56484385
H	15.61716883	-2.07307652	2.90965149
O	12.57562802	-2.30218917	3.35909971
H	11.69214423	-1.91830309	3.44325692
H	13.04731606	-1.70468718	2.75314708

**2) O formation**  
**a. Initial**

C	2.21910731	1.22332431	-0.23782110
C	4.33886160	0.01582983	-0.06885820
C	6.47253238	-1.21456058	-0.08547558
C	8.60214518	-2.44878418	-0.20231057
C	10.72511387	-3.70901669	-0.40091247
C	4.35274511	2.44908079	0.15996923
C	6.46825167	1.24701071	-0.07145758
C	10.01693127	0.01086631	-0.14788792
C	10.72664706	-1.22676029	-0.23088373
C	12.84421639	-2.46448663	-0.27445474
C	6.47867929	3.68826361	-0.23150995
C	8.59829714	2.47827246	-0.07161288
C	10.72760605	1.23981867	-0.11311090
C	12.85217538	0.00631886	-0.21184086
C	14.95414787	-1.20461119	0.00541489
C	8.61630866	4.90968654	0.16035830
C	10.73115043	3.70282798	-0.07498197
C	12.86161374	2.47189934	-0.10401576
C	14.99648590	1.24746478	-0.04446485

C	17.13716385	0.01214628	-0.13685920
C	3.62003308	1.25923204	-0.04904580
C	5.75836672	0.01818388	-0.05823885
C	7.89052417	-1.21584389	-0.14011280
C	10.02189946	-2.46170625	-0.27343730
C	12.14665579	-3.67152130	-0.28883482
C	5.74996725	2.49067297	-0.04550092
C	7.88736684	1.25007508	-0.10210286
C	12.14342008	-1.22674483	-0.26701608
C	14.31882975	-2.47271933	-0.28932464
C	7.87941199	3.72329316	-0.04657941
C	10.01771330	2.47522454	-0.06579743
C	12.15127307	1.23528221	-0.14747734
C	14.28066012	0.00074806	-0.09707373
C	16.36048554	-1.11825455	0.48926408
C	10.01386771	4.94604258	-0.04823368
C	12.15252004	3.70377656	-0.10151477
C	14.28808562	2.46992664	-0.07904097
C	16.41987299	1.24927870	-0.09669225
C	18.47330997	0.00947304	-0.52822632
Cl	17.17757103	-2.75237956	0.56095870
Cl	14.85509222	-2.92031857	-2.13205330
Cl	13.05831952	-5.12266346	-0.01067673
Cl	7.84803940	6.25396838	0.93848931
Cl	5.69430665	5.04738536	-0.96416626
Cl	3.57443417	3.78858404	0.93672042
Cl	1.43695428	2.57651017	-0.98320580
Cl	19.11789387	-1.35279845	-1.37359713
C	8.59832345	0.01609704	-0.12543744
O	16.37796469	-0.60815122	1.86006731
O	15.48385140	-1.44909936	2.68366530
H	16.02193244	-2.26699886	2.75216731
H	13.61717062	-1.56920542	3.23484344

O	12.82078622	-2.12428429	3.30372269
H	12.41562031	-1.87397144	4.14635963
H	14.74933058	-3.31339313	0.25200426

**b. Transition State 1**

C	2.19442925	1.20374959	-0.21809727
C	4.31409147	-0.00964183	-0.07202445
C	6.44728487	-1.24102223	-0.07766138
C	8.57852495	-2.48350819	-0.07262656
C	10.69884862	-3.73847033	-0.21914416
C	4.32997846	2.42856474	0.17026281
C	6.44279334	1.22433852	-0.07056356
C	9.99254621	-0.01638565	-0.12650683
C	10.70184384	-1.25505584	-0.16836584
C	12.81304676	-2.49330100	-0.25398623
C	6.45424951	3.66690411	-0.21311288
C	8.57382570	2.45248755	-0.07022882
C	10.70436040	1.21476899	-0.12939807
C	12.83051618	-0.01906933	-0.27607757
C	14.93467864	-1.23452088	-0.05007363
C	8.59399998	4.88860190	0.17067552
C	10.70639169	3.68048055	-0.08247033
C	12.83656058	2.44411152	-0.15034903
C	14.97167247	1.21584005	-0.05152918
C	17.11335768	-0.02718376	0.11346697
C	3.59603050	1.23617318	-0.03728001
C	5.73418886	-0.00557911	-0.06046871
C	7.86616426	-1.24690307	-0.09147885
C	9.99865318	-2.49163990	-0.13048772
C	12.12231546	-3.69749684	-0.16942273
C	5.72564081	2.46935740	-0.03801481
C	7.86110364	1.22412359	-0.10062668
C	12.11644801	-1.25494238	-0.26715064
C	14.29052497	-2.50799144	-0.30764920



C	7.85608138	3.69942560	-0.03483448
C	9.99399430	2.45174290	-0.07441661
C	12.12683195	1.21120202	-0.20251313
C	14.25896408	-0.02172648	-0.18510891
C	16.28119093	-1.20255679	0.59060076
C	9.99030220	4.92547905	-0.04150311
C	12.12696153	3.67815176	-0.11871415
C	14.26341144	2.44172591	-0.10092640
C	16.39696152	1.21404754	0.05363641
C	18.44751951	-0.02354812	-0.29587186
Cl	17.15729723	-2.79039497	0.70785615
Cl	14.81193196	-2.93607168	-2.09372972
Cl	13.04835727	-5.13064418	0.15538399
Cl	7.82631720	6.22757926	0.95826500
Cl	5.66993954	5.03018811	-0.93857564
Cl	3.55530900	3.76469942	0.95526213
Cl	1.40988674	2.56287022	-0.94985467
Cl	19.10474101	-1.38154994	-1.14757920
C	8.57220821	-0.01220471	-0.10529339
O	15.59615339	-1.01757656	1.83461895
O	16.41861980	-1.06084658	3.27750020
H	16.68247474	-2.00243218	3.24823763
H	14.14031832	-1.59036352	3.40939207
O	13.24384254	-1.86699936	3.13549912
H	12.73704764	-1.89632982	3.96011802
H	14.71956486	-3.32139275	0.27474607

**c. Transition State 2**

C	2.19310978	1.20759061	-0.21553297
C	4.31332620	-0.00731173	-0.07077495
C	6.44849062	-1.23729091	-0.08088374
C	8.58252881	-2.48454079	-0.07554255
C	10.70760629	-3.73360618	-0.22660459
C	4.32940204	2.43240708	0.16708507

C	6.44380287	1.22612465	-0.06940517
C	9.99480380	-0.01340775	-0.12352798
C	10.70902799	-1.25351521	-0.16371457
C	12.81395807	-2.49436399	-0.24536334
C	6.45348333	3.67000604	-0.21044271
C	8.57406084	2.45410752	-0.06938769
C	10.70405273	1.21789534	-0.12807188
C	12.83826535	-0.00870668	-0.28714794
C	14.92151081	-1.23087129	0.09011935
C	8.59285532	4.89222808	0.16783570
C	10.70685616	3.68355156	-0.08071593
C	12.83705150	2.44685736	-0.15580161
C	14.96840441	1.21662407	-0.09324820
C	17.13579472	-0.01675611	0.07218422
C	3.59454721	1.24027733	-0.03708820
C	5.73440848	-0.00176260	-0.06030831
C	7.86710267	-1.24485674	-0.09206771
C	10.00344717	-2.49019331	-0.12854885
C	12.12824186	-3.69659125	-0.16891087
C	5.72544818	2.47204825	-0.03748108
C	7.86166118	1.22611094	-0.09929248
C	12.12017241	-1.25619252	-0.26459202
C	14.29486289	-2.51708148	-0.28892313
C	7.85553295	3.70230101	-0.03429427
C	9.99308904	2.45507918	-0.07373386
C	12.12450706	1.22094022	-0.20809399
C	14.24400908	0.01749560	-0.23754917
C	16.36004368	-1.21570520	0.47616803
C	9.98930855	4.92964190	-0.04112638
C	12.12437668	3.68528954	-0.11600379
C	14.25947831	2.45129949	-0.11717846
C	16.40600473	1.21266548	0.02856284
C	18.47011154	-0.01482099	-0.32035030

Cl	17.19920519	-2.77798926	0.72075346
Cl	14.82220601	-2.85977016	-2.03613460
Cl	13.05138956	-5.13253375	0.15418682
Cl	7.82484780	6.22954854	0.95619603
Cl	5.66936866	5.03208385	-0.93700960
Cl	3.55528525	3.76783545	0.95256998
Cl	1.40822674	2.56687314	-0.94683120
Cl	19.12281495	-1.38210683	-1.15890895
C	8.57451596	-0.01214297	-0.10398389
O	15.40945486	-1.02345278	1.48713529
O	16.37926528	-1.10368545	3.60569037
H	16.72174303	-1.95797175	3.26982473
H	14.16943748	-1.58734654	3.42905335
O	13.27062476	-1.85069524	3.14087083
H	12.75529113	-1.89388758	3.96131936
H	14.71128157	-3.33483880	0.29357005

**d. Transition State 3**

C	2.19294813	1.20463265	-0.21460159
C	4.31384979	-0.01189797	-0.07188035
C	6.44940709	-1.24457014	-0.08282265
C	8.58318694	-2.49489486	-0.09271125
C	10.71064723	-3.73327641	-0.25268576
C	4.32913987	2.42840220	0.16631319
C	6.44396565	1.22102665	-0.06990559
C	9.99439865	-0.01753368	-0.12790076
C	10.70780574	-1.25759403	-0.17260984
C	12.81317829	-2.49784837	-0.24066574
C	6.45321044	3.66628701	-0.20787116
C	8.57414671	2.44958681	-0.06987929
C	10.70425986	1.21391884	-0.12992486
C	12.83856910	-0.01507167	-0.27262913
C	14.92787089	-1.24447382	0.10319671
C	8.59268577	4.88864313	0.16668127

C	10.70772914	3.67953418	-0.08158456
C	12.83941024	2.44106382	-0.15342965
C	14.97102087	1.20428202	-0.09276518
C	17.14594215	-0.03448518	0.00679504
C	3.59454274	1.23614805	-0.03780522
C	5.73504011	-0.00749918	-0.06135073
C	7.86796675	-1.25298004	-0.09653983
C	10.00314499	-2.49511029	-0.14891490
C	12.12874154	-3.69908483	-0.17422765
C	5.72538251	2.46799868	-0.03705497
C	7.86158217	1.22120881	-0.09979890
C	12.11891923	-1.26096403	-0.26141067
C	14.29259270	-2.52305252	-0.28816326
C	7.85544842	3.69803929	-0.03384687
C	9.99318729	2.45126979	-0.07490557
C	12.12533533	1.21645559	-0.20459114
C	14.24174829	0.00806620	-0.21059381
C	16.38713027	-1.24687675	0.39399042
C	9.98946391	4.92626702	-0.04215616
C	12.12540873	3.68072564	-0.11616708
C	14.26194638	2.44252247	-0.11640609
C	16.41203268	1.19616725	-0.00460714
C	18.48123590	-0.01557175	-0.37930783
Cl	17.23967727	-2.80694802	0.57663843
Cl	14.79826923	-2.83191050	-2.04477785
Cl	13.04352476	-5.13771197	0.15788090
Cl	7.82519203	6.22540041	0.95622734
Cl	5.66935275	5.02892582	-0.93348468
Cl	3.55539811	3.76361194	0.95304494
Cl	1.40776843	2.56515433	-0.94298388
Cl	19.15115495	-1.34813096	-1.25793251
C	8.57417710	-0.01823881	-0.10655744
O	15.47996608	-1.10173963	1.46531893

O	15.99685342	-1.32454473	3.90187995
H	16.50693337	-2.02779920	3.44151920
H	14.14470237	-1.63512739	3.28087690
O	13.23795108	-1.86536643	2.96520329
H	12.71854716	-1.91058573	3.78358762
H	14.70948852	-3.34783224	0.28457401

**e. Transition State 4**

C	2.16775389	1.19128012	-0.18969832
C	4.28925384	-0.02414423	-0.06574148
C	6.42315223	-1.25294712	-0.10911313
C	8.55438657	-2.48636107	-0.21295726
C	10.68607294	-3.72264349	-0.36187916
C	4.30262852	2.41427523	0.18463477
C	6.41927336	1.20975408	-0.07256354
C	9.97485433	-0.02474586	-0.19079747
C	10.69266340	-1.26187141	-0.23937489
C	12.78647432	-2.51461594	-0.09765857
C	6.42911593	3.65307126	-0.18595313
C	8.55252443	2.43665904	-0.07345020
C	10.68532073	1.20256541	-0.15237636
C	12.82602519	-0.03040889	-0.21556183
C	14.93432791	-1.25013542	0.25156464
C	8.56655126	4.87340979	0.18396096
C	10.68378078	3.66720331	-0.07763814
C	12.81915466	2.43048218	-0.14851668
C	14.95325247	1.19297158	-0.09268308
C	17.13661441	-0.02476580	-0.15050886
C	3.57043411	1.22100359	-0.02038480
C	5.70923696	-0.01824347	-0.06846720
C	7.83873957	-1.25011958	-0.16925975
C	9.97576277	-2.48743486	-0.27093232
C	12.08329553	-3.70803340	-0.12057107
C	5.69916004	2.45519720	-0.02327720

C	7.83833864	1.21121695	-0.11791092
C	12.10736377	-1.27628420	-0.22751201
C	14.26346336	-2.57571050	0.06888159
C	7.83306220	3.68177906	-0.01984139
C	9.97161413	2.43826440	-0.08332653
C	12.10801933	1.20397022	-0.19620108
C	14.22644008	-0.01279662	-0.11322487
C	16.43343584	-1.22837723	0.34287455
C	9.96338043	4.91264557	-0.02737871
C	12.10196023	3.66931700	-0.11456305
C	14.24087115	2.43080176	-0.12512158
C	16.39473140	1.20116155	-0.10016787
C	18.46523054	0.00205234	-0.55895371
Cl	17.35101547	-2.74027526	0.55353480
Cl	14.93601515	-3.31266127	-1.49682793
Cl	12.89448350	-5.16373734	0.35930246
Cl	7.80085470	6.20544661	0.98422104
Cl	5.64343978	5.02061671	-0.90372942
Cl	3.53210384	3.74614957	0.98035744
Cl	1.38064187	2.55688480	-0.90976102
Cl	19.16027349	-1.29451920	-1.46585412
C	8.55299933	-0.02391601	-0.16803197
O	15.65165764	-1.00284261	1.49661343
O	15.54751626	-1.56792214	4.12119325
H	16.17330195	-1.92275484	3.45713454
H	14.12489279	-1.83393397	3.29484350
O	13.29011520	-2.02919337	2.77381736
H	12.57543094	-1.98488066	3.42546830
H	14.52227110	-3.22529901	0.91241568

**f. Transition State 5**

C	2.17006099	1.19377659	-0.19328361
C	4.29138244	-0.02026231	-0.06623861
C	6.42683730	-1.24900461	-0.11315734

C	8.56138343	-2.48332808	-0.23052284
C	10.69434988	-3.71857433	-0.39533666
C	4.30597569	2.41752805	0.18396996
C	6.42188808	1.21327768	-0.07714622
C	9.97640455	-0.01987295	-0.20256379
C	10.69562720	-1.25579576	-0.24384225
C	12.81326650	-2.50459345	-0.19447014
C	6.43134733	3.65562954	-0.18969152
C	8.55430994	2.43957159	-0.07895886
C	10.68797075	1.20735815	-0.15538823
C	12.82597764	-0.02294469	-0.20367593
C	14.94334066	-1.24901220	0.22414077
C	8.56952820	4.87482401	0.18429091
C	10.68536802	3.67094309	-0.07846806
C	12.82156585	2.43643386	-0.13896018
C	14.95793281	1.20034598	-0.08186477
C	17.14264611	-0.01980140	-0.15155805
C	3.57209356	1.22553992	-0.02192994
C	5.71187430	-0.01468772	-0.07073739
C	7.84250862	-1.24696082	-0.18734274
C	9.97946440	-2.48338676	-0.29005562
C	12.09357686	-3.70521956	-0.19338658
C	5.70132362	2.45925373	-0.02523519
C	7.83978136	1.21388290	-0.12978294
C	12.10645109	-1.26073268	-0.23317654
C	14.25408639	-2.50073815	-0.12845055
C	7.83459759	3.68524802	-0.02228389
C	9.97304684	2.44279382	-0.08550798
C	12.10914114	1.21105859	-0.18765208
C	14.22896762	-0.00288632	-0.08875414
C	16.44038235	-1.21921628	0.35021527
C	9.96518763	4.91644006	-0.02930806
C	12.10386585	3.67375900	-0.11238951

C	14.24322705	2.43650315	-0.11721020
C	16.39923467	1.20504134	-0.10404979
C	18.46733157	0.00491540	-0.57223124
Cl	17.36649519	-2.73191017	0.57008461
Cl	15.00064623	-3.35759862	-1.46599823
Cl	12.91329314	-5.14493668	0.33267524
Cl	7.80340787	6.20594388	0.98481415
Cl	5.64534636	5.02349562	-0.90441620
Cl	3.53407727	3.74904435	0.97819527
Cl	1.38111177	2.55929324	-0.91129023
Cl	19.15908488	-1.29925716	-1.47116888
C	8.55419129	-0.02100501	-0.19032649
O	15.66881337	-1.00429330	1.49866449
O	15.27335092	-1.71229604	4.10641285
H	16.06209402	-1.94049970	3.58966720
H	14.52749946	-1.80786748	3.43375696
O	13.49481701	-2.28949178	2.27811810
H	12.85429269	-2.56491776	2.95977842
H	13.99252763	-3.01081145	1.66572922

**g. Final**

C	2.16968140	1.19532751	-0.19705098
C	4.29087300	-0.01907416	-0.06768892
C	6.42752835	-1.24964445	-0.09003490
C	8.56551308	-2.49017063	-0.13380958
C	10.69376310	-3.73149379	-0.32278110
C	4.30531125	2.41769133	0.18414412
C	6.42075404	1.21424274	-0.06639115
C	9.97761153	-0.02411985	-0.10491536
C	10.69829177	-1.26253325	-0.14536273
C	12.82603726	-2.51510120	-0.31596926
C	6.42976862	3.65646086	-0.19527510
C	8.55154957	2.44337495	-0.06193642
C	10.68149330	1.20900806	-0.10815613



C	12.81532243	-0.01802241	-0.27536986
C	14.92021466	-1.27635495	-0.10911477
C	8.56692240	4.87874499	0.18335193
C	10.68222699	3.67415788	-0.07495971
C	12.81642627	2.43906493	-0.15610248
C	14.95129490	1.20214906	-0.15709029
C	17.12494740	-0.03134462	-0.12356067
C	3.57161465	1.22648171	-0.02367090
C	5.71200041	-0.01457339	-0.06116812
C	7.84634559	-1.25194263	-0.10435942
C	9.98249251	-2.49472669	-0.18973875
C	12.09850922	-3.72148362	-0.20969764
C	5.70013547	2.46017725	-0.02747272
C	7.83936424	1.21542710	-0.09525630
C	12.10669861	-1.26103055	-0.23922530
C	14.21458979	-2.47178680	-0.52504448
C	7.83186940	3.68866669	-0.02239361
C	9.96929258	2.44645658	-0.06556233
C	12.09961848	1.21465543	-0.19130398
C	14.22341071	0.00342051	-0.28688413
C	16.36817332	-1.25939289	0.24446393
C	9.96229457	4.91968109	-0.02966200
C	12.10066229	3.67642531	-0.11396329
C	14.23844303	2.43916205	-0.13801717
C	16.38935367	1.19876829	-0.08977036
C	18.46188647	-0.00671714	-0.50164890
Cl	17.30263402	-2.77058205	0.47200884
Cl	15.00311065	-3.63302918	-1.51822279
Cl	12.93298926	-5.13447500	0.33255795
Cl	7.79844044	6.21301520	0.97717708
Cl	5.64333093	5.02312292	-0.91413163
Cl	3.53569265	3.75018209	0.97983930
Cl	1.38412958	2.56246233	-0.91541728

Cl	19.15991072	-1.29272857	-1.42892414
C	8.55489090	-0.02211990	-0.10007314
O	15.47768804	-1.13926151	1.32319796
O	15.86379821	-1.44084376	4.09824771
H	16.23646941	-1.84587408	3.29795869
H	14.90356773	-1.56434079	3.96553049
O	13.12914623	-1.97103102	3.20711241
H	12.27658673	-1.76968309	3.62017732
H	13.13980613	-1.45750200	2.38360234

**3) OH formation**  
**a. Initial**

C	2.16664643	1.19104678	-0.19508647
C	4.28719005	-0.02289327	-0.06204362
C	6.42192827	-1.25398233	-0.08347830
C	8.55374611	-2.49344710	-0.15792151
C	10.68079630	-3.71893502	-0.43353487
C	4.30042708	2.41426608	0.18384090
C	6.41530339	1.21056171	-0.06467847
C	9.96926330	-0.02341230	-0.12844582
C	10.68539522	-1.25977849	-0.20481246
C	12.78334904	-2.50958461	-0.32141474
C	6.42650600	3.65298007	-0.19123445
C	8.54791677	2.43932492	-0.06265270
C	10.67711311	1.20571297	-0.11240424
C	12.81628660	-0.02472022	-0.25353800
C	14.92970345	-1.27245366	-0.02511240
C	8.56349105	4.87460158	0.18175910
C	10.67983388	3.66967305	-0.07219344
C	12.81475966	2.43316301	-0.12998053
C	14.94933569	1.19226077	-0.11020544
C	17.12896559	-0.03662090	-0.22416940
C	3.56863346	1.22129847	-0.02159678
C	5.70728201	-0.01846505	-0.05773771

C	7.83901473	-1.25526853	-0.11050385
C	9.97426592	-2.49002972	-0.24962068
C	12.09646711	-3.70771981	-0.34528142
C	5.69605443	2.45559225	-0.02505242
C	7.83428737	1.21273903	-0.09575973
C	12.09486460	-1.26964852	-0.27720021
C	14.25646025	-2.52778311	-0.46221339
C	7.82947422	3.68358972	-0.02112244
C	9.96620040	2.44161488	-0.06656304
C	12.09937559	1.20783193	-0.17227456
C	14.22026099	-0.00345670	-0.21831758
C	16.40397850	-1.28766020	0.10902487
C	9.96022961	4.91423045	-0.02930188
C	12.09830793	3.67200460	-0.10416243
C	14.23790572	2.43133080	-0.10822664
C	16.39132861	1.19040818	-0.09926522
C	18.44839315	0.01774370	-0.65797022
Cl	17.25568773	-2.84915292	0.03439284
Cl	14.61977067	-2.65821780	-2.27898744
Cl	12.99635332	-5.17771412	-0.12346957
Cl	7.79556221	6.21092896	0.97684651
Cl	5.64021299	5.01962080	-0.91422196
Cl	3.52838621	3.74886797	0.97748429
Cl	1.38082094	2.55724199	-0.91957271
Cl	19.10251743	-1.20177967	-1.70432020
C	8.54860638	-0.02362708	-0.10974022
O	15.60979628	-1.23615668	1.29728138
H	14.31217933	-2.09429442	2.55842719
O	13.43739084	-2.51218173	2.62734451
H	12.95142927	-1.95785212	3.25678807
H	14.71842898	-3.40757114	-0.01543593

**b. Transition State 1**

C	2.16321124	1.18105715	-0.19844559
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C	4.28245213	-0.03094652	-0.05994454
C	6.41331851	-1.26089481	-0.08716003
C	8.53999910	-2.48871931	-0.18843713
C	10.65773849	-3.73226282	-0.43155674
C	4.29315403	2.40851613	0.18343018
C	6.40708678	1.20478384	-0.06565500
C	9.95978421	-0.03108498	-0.15176630
C	10.67038958	-1.26710996	-0.23775302
C	12.77160815	-2.51900707	-0.28608692
C	6.42168545	3.64782399	-0.19205107
C	8.54169713	2.43370298	-0.06368340
C	10.67100628	1.19407111	-0.11711658
C	12.80875350	-0.04692297	-0.23205046
C	14.93534941	-1.26351126	-0.04196903
C	8.55866639	4.86838871	0.18336704
C	10.67409600	3.65787901	-0.07072495
C	12.80931424	2.42033033	-0.11865879
C	14.95343331	1.18962978	-0.07553286
C	17.10650023	-0.03914820	-0.12305873
C	3.56541567	1.21269458	-0.02009851
C	5.70028271	-0.02634773	-0.05721321
C	7.82792096	-1.25634939	-0.13374472
C	9.96064032	-2.49389696	-0.28114121
C	12.07175511	-3.72034812	-0.30280612
C	5.68914493	2.44992534	-0.02457676
C	7.82692321	1.20871634	-0.10068391
C	12.08488941	-1.27944280	-0.28084975
C	14.25431244	-2.55348257	-0.24991167
C	7.82473715	3.67777324	-0.02000342
C	9.96077691	2.43043570	-0.06723162
C	12.09544757	1.18759764	-0.16081770
C	14.23603005	-0.04856813	-0.14629117
C	16.34347574	-1.20884383	0.50517075

C	9.95574742	4.90334490	-0.02821828
C	12.09544285	3.65809672	-0.10214277
C	14.23812994	2.41637368	-0.09739727
C	16.38178136	1.19867701	-0.07886125
C	18.40554306	-0.01130687	-0.59212655
Cl	17.21998565	-2.87042274	0.42517044
Cl	14.86783969	-3.13841736	-1.90796461
Cl	12.95040878	-5.17585271	0.02224287
Cl	7.79395927	6.20672642	0.97411762
Cl	5.63771074	5.01224658	-0.91755653
Cl	3.51796102	3.74281289	0.97080078
Cl	1.37919529	2.54037119	-0.93142715
Cl	19.05464960	-1.32221432	-1.51119582
C	8.53984202	-0.02536911	-0.12779960
O	16.09652030	-0.92228094	1.79010094
H	14.79226413	-1.80327487	2.39894380
O	13.93248353	-2.30352283	2.46530293
H	13.34597911	-1.75621830	2.99832476
H	14.60687868	-3.29480461	0.46933632

**c. Transition State 2**

C	2.16353747	1.18246446	-0.19745947
C	4.28285752	-0.02902694	-0.05918506
C	6.41332975	-1.25823216	-0.08605073
C	8.53870360	-2.48632260	-0.18695018
C	10.65230731	-3.73095101	-0.43968720
C	4.29376203	2.40987437	0.18381377
C	6.40750277	1.20658891	-0.06563576
C	9.95849855	-0.02891428	-0.14989373
C	10.66648128	-1.26487590	-0.24359024
C	12.76500960	-2.51505600	-0.33425491
C	6.42205550	3.64895240	-0.19262761
C	8.54194024	2.43517538	-0.06368142
C	10.67010191	1.19637978	-0.11611402

C	12.80694145	-0.04319308	-0.23522845
C	14.93413293	-1.25617374	-0.07694452
C	8.55898828	4.86943643	0.18359726
C	10.67447968	3.65972147	-0.07004478
C	12.80885532	2.42318895	-0.11692218
C	14.95273452	1.19520086	-0.07156570
C	17.10440072	-0.03558278	-0.11601702
C	3.56576726	1.21425539	-0.01926387
C	5.70056211	-0.02422457	-0.05704762
C	7.82770754	-1.25399664	-0.13228771
C	9.95826103	-2.49208981	-0.28570962
C	12.06646478	-3.71901011	-0.32016105
C	5.68968356	2.45125571	-0.02481103
C	7.82700934	1.21056193	-0.10046079
C	12.08031656	-1.27648262	-0.29649988
C	14.24254745	-2.54106433	-0.21958735
C	7.82494390	3.67893963	-0.02029529
C	9.96086250	2.43238758	-0.06669313
C	12.09414564	1.19133009	-0.15781946
C	14.23402533	-0.04148373	-0.14964216
C	16.33969121	-1.20546435	0.49915501
C	9.95617537	4.90488453	-0.02725196
C	12.09550133	3.66033823	-0.10089440
C	14.23748176	2.42020921	-0.09510316
C	16.38035650	1.20236846	-0.07406912
C	18.40138500	-0.01168095	-0.58924949
Cl	17.23870204	-2.83782992	0.47978702
Cl	14.96744376	-3.38335055	-1.67834505
Cl	12.93219214	-5.16578073	0.06224850
Cl	7.79354339	6.20758111	0.97373507
Cl	5.63797069	5.01300390	-0.91854793
Cl	3.51891107	3.74470069	0.97073036
Cl	1.37938610	2.54178977	-0.93046389

Cl	19.05041809	-1.32557140	-1.50448999
C	8.53943113	-0.02327521	-0.12628031
O	16.05346142	-0.90805586	1.78020139
H	14.94684258	-1.87626044	2.37821793
O	14.17686352	-2.52152226	2.48877725
H	13.40510408	-1.98508176	2.71117676
H	14.41223221	-3.02662746	0.79325917

**d. Transition State 3**

C	2.16274771	1.18250412	-0.19624856
C	4.28142451	-0.02964909	-0.05957704
C	6.41127436	-1.26096281	-0.08684621
C	8.53674962	-2.49112152	-0.18325275
C	10.64996797	-3.73802292	-0.43924755
C	4.29331754	2.40894098	0.18316613
C	6.40689993	1.20518254	-0.06620322
C	9.95647699	-0.03011558	-0.14706790
C	10.66408296	-1.26787221	-0.23730918
C	12.77242684	-2.51654423	-0.36079790
C	6.42148675	3.64822486	-0.19202154
C	8.54069981	2.43415322	-0.06391312
C	10.66877641	1.19652093	-0.11692432
C	12.80276340	-0.04173125	-0.22748976
C	14.91709560	-1.27681414	-0.11042093
C	8.55870326	4.86869665	0.18292770
C	10.67357211	3.65967976	-0.07075311
C	12.80664037	2.42306535	-0.11828671
C	14.94778548	1.18946146	-0.05210066
C	17.09430346	-0.04587628	-0.09237824
C	3.56467585	1.21412094	-0.01969067
C	5.69897651	-0.02539120	-0.05836867
C	7.82627776	-1.25659428	-0.13105779
C	9.95518570	-2.49452406	-0.28515110
C	12.06037926	-3.72620322	-0.33723501

C	5.68918651	2.45063713	-0.02505890
C	7.82584543	1.20939309	-0.10118250
C	12.07872205	-1.27349589	-0.28479968
C	14.22875431	-2.48497981	-0.36581407
C	7.82413333	3.67831239	-0.02049986
C	9.95918815	2.43297375	-0.06762873
C	12.09030636	1.19508087	-0.16039189
C	14.22131222	-0.04248268	-0.11610166
C	16.31382277	-1.22296882	0.50692926
C	9.95520684	4.90531406	-0.02803670
C	12.09347967	3.66111738	-0.10140914
C	14.23386387	2.41830963	-0.09335728
C	16.37512869	1.19678658	-0.06174101
C	18.39240898	-0.02214886	-0.57269051
Cl	17.22861788	-2.84676131	0.47588593
Cl	14.98279316	-3.46129656	-1.64194055
Cl	12.93384352	-5.16994909	0.06046685
Cl	7.79261162	6.20735894	0.97340268
Cl	5.63688082	5.01316277	-0.91819892
Cl	3.51834475	3.74454749	0.97052580
Cl	1.37842293	2.54251672	-0.93056073
Cl	19.04395206	-1.32924392	-1.50055974
C	8.53832070	-0.02576976	-0.12610946
O	16.02059351	-0.96031947	1.81533882
H	15.07812230	-1.81261613	2.25719709
O	14.24057940	-2.59172330	2.32428300
H	13.44838982	-2.07173565	2.57919369
H	14.28538658	-2.83767206	1.15107337

**e. Transition State 4**

C	2.16641606	1.19687498	-0.19380973
C	4.28822701	-0.01441864	-0.05586293
C	6.42346545	-1.24651245	-0.08153600
C	8.55714391	-2.47274703	-0.19157175



C	10.69093233	-3.71542717	-0.44519017
C	4.30135581	2.42119096	0.18316768
C	6.41649399	1.21751632	-0.06544706
C	9.97223773	-0.01626336	-0.13402516
C	10.68903474	-1.25213494	-0.23067217
C	12.82839028	-2.47278405	-0.46189598
C	6.42670186	3.65863862	-0.19431851
C	8.54806848	2.44745037	-0.06115501
C	10.67966579	1.21479748	-0.10235625
C	12.81585457	-0.01212111	-0.19615007
C	14.94056432	-1.26223611	-0.16316157
C	8.56330275	4.88147584	0.18348946
C	10.67950607	3.67739036	-0.06426826
C	12.81400971	2.44372281	-0.09595553
C	14.95679395	1.20611586	-0.02336752
C	17.12141843	-0.00994801	-0.11815187
C	3.56939209	1.22818322	-0.01990870
C	5.70807884	-0.01165496	-0.05621531
C	7.84073658	-1.24075154	-0.13002085
C	9.97825199	-2.47827657	-0.29230519
C	12.10674017	-3.69056319	-0.39221350
C	5.69686109	2.46153566	-0.02587385
C	7.83565183	1.22142757	-0.09781480
C	12.10760149	-1.24365508	-0.29335286
C	14.26499171	-2.39125117	-0.60511875
C	7.82932630	3.69050929	-0.02088346
C	9.96710700	2.44995627	-0.06132157
C	12.10013119	1.21979678	-0.12916136
C	14.22704644	-0.02266950	-0.08944507
C	16.33034385	-1.16764573	0.46732741
C	9.95970037	4.92113822	-0.02495836
C	12.09878332	3.67932820	-0.09197701
C	14.24092495	2.43560510	-0.07015512

C	16.38981302	1.22094758	-0.07415719
C	18.43872450	-0.00412300	-0.55053976
Cl	17.21143460	-2.76709351	0.56928894
Cl	15.08561807	-3.60302882	-1.53573060
Cl	12.95992707	-5.12721591	0.09336045
Cl	7.79269328	6.21823971	0.97457630
Cl	5.64082195	5.02330995	-0.92118617
Cl	3.52788124	3.75690646	0.97331185
Cl	1.38133580	2.55966610	-0.92494702
Cl	19.08448810	-1.34654728	-1.43708956
C	8.55139812	-0.01269290	-0.11990059
O	16.11075465	-0.76139043	1.80679506
H	15.43312180	-1.39786532	2.19437230
O	14.17122745	-2.46501289	2.51301499
H	13.34458846	-2.00362377	2.71264123
H	14.02231734	-2.87107454	1.64090348

**f. Transition State 5**

C	2.16804353	1.19863569	-0.18859125
C	4.29047114	-0.01313844	-0.05491291
C	6.42619512	-1.24638545	-0.08004780
C	8.56052349	-2.47624924	-0.18289428
C	10.69667298	-3.72007060	-0.42616543
C	4.30493794	2.42248651	0.18442054
C	6.41962692	1.21773383	-0.06554913
C	9.97534629	-0.01775875	-0.13553488
C	10.69214002	-1.25415774	-0.23367273
C	12.83012497	-2.47458779	-0.47244934
C	6.42927262	3.65938690	-0.19368647
C	8.55030006	2.44788959	-0.05993194
C	10.68114088	1.21490898	-0.10251056
C	12.81467913	-0.01227848	-0.20254474
C	14.93202441	-1.26294606	-0.17886178
C	8.56501251	4.88253966	0.18701558

C	10.68119111	3.67878723	-0.06212333
C	12.81526055	2.44468258	-0.09468147
C	14.95637471	1.20598022	-0.02497416
C	17.11966479	-0.01591187	-0.10033890
C	3.57150945	1.22989676	-0.01771148
C	5.71071171	-0.01096053	-0.05589857
C	7.84396364	-1.24258611	-0.12724487
C	9.98228436	-2.48183176	-0.28584896
C	12.11327275	-3.69246183	-0.38379801
C	5.70005080	2.46203845	-0.02616896
C	7.83869496	1.22109732	-0.09747019
C	12.11030216	-1.24576069	-0.30405861
C	14.26302994	-2.39617561	-0.61090498
C	7.83153186	3.69136562	-0.01916268
C	9.96914426	2.45068295	-0.05991793
C	12.10105028	1.22030411	-0.12934083
C	14.22517230	-0.02085795	-0.09804755
C	16.30811690	-1.17961938	0.44977585
C	9.96145076	4.92281484	-0.02101600
C	12.10040466	3.68080042	-0.09077679
C	14.24176947	2.43702902	-0.06897039
C	16.38898699	1.21859663	-0.06972308
C	18.44512316	-0.01226588	-0.50876108
Cl	17.18457696	-2.74716349	0.63040391
Cl	15.10820522	-3.62584276	-1.49642241
Cl	12.96868209	-5.11323543	0.12337948
Cl	7.79259767	6.21784438	0.98005002
Cl	5.64414403	5.02469376	-0.92085987
Cl	3.53553871	3.75898593	0.97834228
Cl	1.38152619	2.56540053	-0.91131636
Cl	19.10079406	-1.38107711	-1.35384675
C	8.55438907	-0.01388520	-0.11941904
O	15.96725545	-0.80668945	1.81856186

H	16.58922777	-1.28200037	2.39294317
O	13.47083676	-2.68185523	2.64932520
H	13.34160699	-1.75747205	2.91716673
H	14.07148684	-2.60013054	1.89285799

**g. Final**

C	2.17896342	1.20314382	-0.20594106
C	4.30062860	-0.00858264	-0.06127323
C	6.43597535	-1.24189797	-0.07823973
C	8.56975121	-2.47157807	-0.17915207
C	10.70540705	-3.71437175	-0.42390197
C	4.31599723	2.42779656	0.17073456
C	6.43047443	1.22207620	-0.06977286
C	9.98476292	-0.01281601	-0.12928697
C	10.70154228	-1.24918580	-0.22513615
C	12.84302652	-2.47077062	-0.44966314
C	6.43980881	3.66428871	-0.20513737
C	8.56041874	2.45302124	-0.06383592
C	10.69158895	1.21967206	-0.09961169
C	12.82517947	-0.00924376	-0.18712002
C	14.94183967	-1.26216305	-0.14167054
C	8.57740590	4.88884720	0.17253868
C	10.69238412	3.68282922	-0.06851437
C	12.82478017	2.44877589	-0.09218678
C	14.96417526	1.21031273	-0.01423357
C	17.12810982	-0.01072151	-0.09575773
C	3.58186456	1.23526183	-0.03076388
C	5.72097418	-0.00618155	-0.05823436
C	7.85381983	-1.23813889	-0.12341330
C	9.99116085	-2.47660821	-0.28120406
C	12.12254683	-3.68793025	-0.37146861
C	5.71168640	2.46623810	-0.03564206
C	7.84897066	1.22575609	-0.09830031
C	12.12084741	-1.24229849	-0.28792006

C	14.27663045	-2.39720442	-0.57066404
C	7.84184868	3.69740538	-0.02883738
C	9.97967038	2.45556606	-0.06207428
C	12.11188980	1.22353813	-0.12310642
C	14.23531002	-0.01909150	-0.07906061
C	16.32594911	-1.17540080	0.46840151
C	9.97374322	4.92686764	-0.03467382
C	12.11094999	3.68481443	-0.09357095
C	14.25074630	2.44153662	-0.06438022
C	16.39691028	1.22393556	-0.06366282
C	18.45337020	-0.00635881	-0.51041686
Cl	17.22298957	-2.73665472	0.65029066
Cl	15.12503167	-3.62970010	-1.44367977
Cl	12.96511175	-5.11381103	0.13951466
Cl	7.80573540	6.22786982	0.96016625
Cl	5.65525913	5.02722805	-0.93675897
Cl	3.54291901	3.76554943	0.95885516
Cl	1.39467706	2.56579776	-0.93873833
Cl	19.10453545	-1.36722847	-1.36790728
C	8.56392870	-0.00934481	-0.11575369
O	15.99015825	-0.80900984	1.83502403
H	16.82188660	-0.80411386	2.34650389
O	13.49603917	-2.50478623	2.81657351
H	12.91826843	-1.77684457	3.08885183
H	14.32210524	-2.05911003	2.55593769

#### 4) HOH formation

##### a. Initial

C	2.17828156	1.19972973	-0.19663272
C	4.29930576	-0.01040062	-0.05977479
C	6.43451754	-1.23797440	-0.09101384
C	8.56692984	-2.47232687	-0.18934649
C	10.69678764	-3.73411409	-0.35202178
C	4.31420053	2.42513950	0.18564933

C	6.42815256	1.22298578	-0.06955447
C	9.98072033	-0.01543515	-0.16815357
C	10.69579023	-1.25313897	-0.23923627
C	12.81554969	-2.48737041	-0.27252939
C	6.43773251	3.66349948	-0.19302380
C	8.55980643	2.45026627	-0.06866503
C	10.69002573	1.21446279	-0.12913701
C	12.82078818	-0.01364692	-0.22293120
C	14.92841549	-1.22279802	0.03125852
C	8.57697725	4.88446368	0.18279336
C	10.69093560	3.67897060	-0.07256389
C	12.82365405	2.44798074	-0.11440018
C	14.96305343	1.22383701	-0.03541575
C	17.11088460	-0.01203083	-0.04083643
C	3.58005433	1.23249238	-0.02061478
C	5.71944605	-0.00475034	-0.06139399
C	7.85141345	-1.23841277	-0.14752078
C	9.98937550	-2.48697195	-0.26093071
C	12.11920617	-3.69358709	-0.25634145
C	5.70885302	2.46649892	-0.02505656
C	7.84663363	1.22412698	-0.10748596
C	12.11248557	-1.25208354	-0.27327855
C	14.29714760	-2.49431448	-0.28421446
C	7.84099490	3.69505553	-0.02239699
C	9.97877931	2.45064639	-0.07309375
C	12.11309298	1.21491013	-0.16315871
C	14.24647430	-0.01554252	-0.09500812
C	16.31047800	-1.14238679	0.60496677
C	9.97345893	4.92287309	-0.02903621
C	12.11081660	3.68093388	-0.10166981
C	14.25039903	2.44694115	-0.08395029
C	16.39160157	1.22640683	-0.06121709
C	18.44098978	-0.01924257	-0.44701433

Cl	17.13843664	-2.75844828	0.68235374
Cl	14.85246711	-2.91650546	-2.08727555
Cl	13.03536278	-5.13945985	0.04092903
Cl	7.81070069	6.22015824	0.98071784
Cl	5.65123189	5.03090046	-0.91176387
Cl	3.54243230	3.75789779	0.98247159
Cl	1.39287530	2.56512102	-0.91961729
Cl	19.08610295	-1.39908446	-1.27154883
C	8.56007247	-0.01040558	-0.14301318
O	16.10467055	-0.74172204	1.98633392
H	16.98651976	-0.70283489	2.39943949
H	14.53721707	-1.76993238	2.57308532
O	13.74769976	-2.34319547	2.62818233
H	13.16169149	-1.89046938	3.25272710
H	14.71321140	-3.33056951	0.27332698

**b. Transition State 1**

C	2.17092486	1.19076608	-0.20924783
C	4.28898003	-0.02087511	-0.06186583
C	6.41783027	-1.25119343	-0.09305015
C	8.54488064	-2.47203652	-0.21983385
C	10.66565524	-3.72395992	-0.37963424
C	4.30452465	2.41558328	0.17771121
C	6.41657721	1.21371523	-0.06834896
C	9.96843855	-0.02310935	-0.15744850
C	10.67832880	-1.25844195	-0.24002040
C	12.78768164	-2.51678992	-0.22423802
C	6.43123097	3.65422606	-0.20690449
C	8.55064953	2.44216125	-0.06563952
C	10.68055703	1.20362189	-0.11661755
C	12.81080420	-0.03815306	-0.25095482
C	14.93794223	-1.25020423	-0.06339863
C	8.56877505	4.87562056	0.17676183
C	10.68136674	3.66910548	-0.07268244

C	12.81262255	2.43260161	-0.12220912
C	14.95301070	1.20390516	-0.11326162
C	17.09488306	-0.01327264	-0.14002669
C	3.57202795	1.22269736	-0.02724462
C	5.70714621	-0.01671717	-0.05737486
C	7.83353555	-1.24334516	-0.15027470
C	9.96469299	-2.48310515	-0.27879128
C	12.07099597	-3.70664678	-0.17051629
C	5.69935095	2.45838974	-0.03334939
C	7.83604085	1.21650079	-0.10218059
C	12.09790763	-1.27143374	-0.27892567
C	14.27029156	-2.56133230	-0.10142169
C	7.83312077	3.68627291	-0.02841602
C	9.97055466	2.44011663	-0.06560354
C	12.10482302	1.19458858	-0.16526245
C	14.24835817	-0.05183615	-0.19252182
C	16.31483842	-1.13605960	0.46569355
C	9.96448862	4.91381860	-0.03600260
C	12.10276301	3.66629342	-0.10334750
C	14.23968050	2.42733047	-0.10886672
C	16.37392532	1.22192415	-0.13069826
C	18.43034407	-0.00505462	-0.54174844
Cl	17.19409943	-2.66574383	0.65055391
Cl	14.95129629	-3.54748320	-1.56815762
Cl	12.86638160	-5.13842998	0.39584041
Cl	7.80069983	6.21516576	0.96119881
Cl	5.64915538	5.01575998	-0.93888190
Cl	3.53045584	3.75319154	0.95932735
Cl	1.38876257	2.54904961	-0.94676842
Cl	19.12831178	-1.32822164	-1.41096034
C	8.54725058	-0.01602710	-0.13251515
O	16.04611988	-0.60051203	1.99455408
H	16.76799430	-0.92944957	2.56458340



H	14.68126155	-1.51406934	2.55598570
O	13.99781577	-2.22122046	2.65283379
H	13.21888286	-1.79689584	3.04061400
H	14.53948256	-3.13933999	0.78861037

**c. Transition State 2**

C	2.16955049	1.19089300	-0.20905358
C	4.28733459	-0.02254029	-0.06200677
C	6.41455793	-1.25423627	-0.09246402
C	8.53940650	-2.47977582	-0.22093089
C	10.66291034	-3.72617033	-0.37115468
C	4.30279804	2.41601398	0.17469182
C	6.41523629	1.21201301	-0.06771870
C	9.96564719	-0.02468365	-0.15265291
C	10.67386619	-1.26072587	-0.23490020
C	12.77935996	-2.51930523	-0.22641462
C	6.43012733	3.65385359	-0.20644174
C	8.54965177	2.43989102	-0.06571010
C	10.67911872	1.20166959	-0.11238628
C	12.81156044	-0.04085921	-0.24406092
C	14.95031430	-1.25860718	-0.12369476
C	8.56717203	4.87566740	0.17371203
C	10.68019571	3.66793265	-0.07213229
C	12.81144730	2.43046961	-0.11852414
C	14.94334581	1.19705866	-0.14184071
C	17.07797637	-0.02551999	-0.23789478
C	3.57043214	1.22278770	-0.02818436
C	5.70531545	-0.01824193	-0.05679678
C	7.83124976	-1.24820921	-0.14519341
C	9.95874076	-2.48554155	-0.27308026
C	12.06783628	-3.70853565	-0.16068882
C	5.69824662	2.45767792	-0.03418211
C	7.83430758	1.21456510	-0.10053980
C	12.09212602	-1.27426148	-0.27735541

C	14.25841201	-2.56941525	-0.09663852
C	7.83219636	3.68513651	-0.02920229
C	9.96916805	2.43854255	-0.06492597
C	12.10301357	1.19335023	-0.15668355
C	14.24287736	-0.04433848	-0.22140309
C	16.33736004	-1.20875837	0.11137783
C	9.96314947	4.91368884	-0.03716778
C	12.10017956	3.66714456	-0.10135697
C	14.23306869	2.42895323	-0.11197212
C	16.35841223	1.21197360	-0.17803717
C	18.43903482	0.00585775	-0.57645287
Cl	17.18579072	-2.64069865	0.57901126
Cl	14.93545972	-3.60662197	-1.49541039
Cl	12.85250731	-5.13474229	0.42138544
Cl	7.79950588	6.21443313	0.95847870
Cl	5.64886141	5.01533792	-0.93888104
Cl	3.52996503	3.75355564	0.95647885
Cl	1.38760347	2.54971051	-0.94537673
Cl	19.15151240	-1.30805839	-1.44474417
C	8.54516728	-0.01978879	-0.12785761
O	15.92820877	-0.45113718	2.27493855
H	16.67960248	-0.87823518	2.72807075
H	14.76292414	-1.47392603	2.56911606
O	14.08044072	-2.23295736	2.64925950
H	13.24417685	-1.83589880	2.91478847
H	14.48636415	-3.05216749	0.86693111

**d. Transition State 3**

C	2.16855717	1.19254926	-0.20852744
C	4.28598103	-0.02110088	-0.06173405
C	6.41207977	-1.25273801	-0.09252167
C	8.53662842	-2.47966809	-0.22016083
C	10.66042531	-3.72213804	-0.37371251
C	4.30200803	2.41764519	0.17282741

C	6.41428445	1.21293883	-0.06740574
C	9.96321255	-0.02266211	-0.14890471
C	10.67040455	-1.25855957	-0.23326176
C	12.77519736	-2.51671949	-0.24382929
C	6.42947429	3.65483400	-0.20603808
C	8.54836899	2.44072638	-0.06505832
C	10.67754458	1.20330063	-0.10941866
C	12.81118186	-0.03791989	-0.24447426
C	14.95591433	-1.26112400	-0.18018281
C	8.56604965	4.87715959	0.17203549
C	10.67872171	3.66953964	-0.07120338
C	12.80893815	2.43271302	-0.11731574
C	14.94030963	1.19943867	-0.15480325
C	17.07225879	-0.02621555	-0.26962616
C	3.56916963	1.22465208	-0.02875185
C	5.70341656	-0.01648021	-0.05663464
C	7.82910738	-1.24700217	-0.14328949
C	9.95493294	-2.48302287	-0.27237018
C	12.06440776	-3.70647411	-0.16178024
C	5.69738961	2.45885044	-0.03472135
C	7.83279038	1.21583771	-0.09941025
C	12.08756908	-1.27180550	-0.27984196
C	14.24937952	-2.55921467	-0.09032093
C	7.83125248	3.68634053	-0.02944422
C	9.96754721	2.44022224	-0.06395422
C	12.10083473	1.19630063	-0.15259978
C	14.24013059	-0.03658153	-0.24062416
C	16.34089621	-1.22919380	-0.01263090
C	9.96185226	4.91567155	-0.03759866
C	12.09768727	3.67001282	-0.09971909
C	14.22881024	2.43251666	-0.11468908
C	16.35630934	1.21159237	-0.18108186
C	18.43881373	0.01352137	-0.58910563

Cl	17.18619389	-2.62389449	0.55102037
Cl	14.94748701	-3.69669828	-1.37141646
Cl	12.83471860	-5.12533912	0.45794267
Cl	7.79849122	6.21538847	0.95681701
Cl	5.64851855	5.01600755	-0.93910787
Cl	3.53003262	3.75505687	0.95514484
Cl	1.38680519	2.55152717	-0.94468043
Cl	19.16363536	-1.29515162	-1.45532000
C	8.54343359	-0.01896056	-0.12543095
O	15.85188136	-0.45879941	2.44158098
H	16.67348649	-0.87231445	2.75537845
H	14.90714021	-1.45782775	2.57836106
O	14.20920076	-2.29680550	2.64845616
H	13.31637091	-1.93961703	2.73324400
H	14.41560756	-2.90719734	0.98033384

**e. Transition State 4**

C	2.16932418	1.19227546	-0.20824106
C	4.28624909	-0.02118955	-0.06161411
C	6.41264068	-1.25368824	-0.09295251
C	8.53782398	-2.48326789	-0.22477234
C	10.66519841	-3.72543229	-0.37284928
C	4.30284648	2.41699112	0.17219844
C	6.41485568	1.21260364	-0.06775323
C	9.96355935	-0.02316079	-0.14844432
C	10.67120857	-1.25993304	-0.22873788
C	12.78596252	-2.51651892	-0.25057017
C	6.43037328	3.65433153	-0.20586367
C	8.54825841	2.44059958	-0.06501409
C	10.67856725	1.20319598	-0.11007735
C	12.81299058	-0.03881395	-0.24042755
C	14.95385676	-1.27117604	-0.18642983
C	8.56703691	4.87652757	0.17149564
C	10.67945895	3.66943155	-0.07151546

C	12.80939965	2.43209634	-0.11717736
C	14.94101127	1.19728554	-0.15393292
C	17.07105247	-0.03349186	-0.27478965
C	3.56956033	1.22458504	-0.02882991
C	5.70372619	-0.01670696	-0.05726179
C	7.82961032	-1.24855757	-0.14376814
C	9.95578064	-2.48360567	-0.27338917
C	12.06519768	-3.71144722	-0.16899839
C	5.69823473	2.45862212	-0.03511104
C	7.83319284	1.21559376	-0.09964001
C	12.08876253	-1.26964543	-0.27031987
C	14.23783347	-2.53418695	-0.16087529
C	7.83178029	3.68603022	-0.02984887
C	9.96790954	2.44059750	-0.06430535
C	12.10000706	1.19897110	-0.15422571
C	14.23801141	-0.03610015	-0.22795328
C	16.34612674	-1.23373137	-0.03248772
C	9.96234501	4.91586185	-0.03815569
C	12.09797440	3.67037523	-0.09919910
C	14.22938024	2.43221336	-0.11389312
C	16.35607420	1.20679644	-0.19928783
C	18.44337379	0.01028573	-0.58506947
Cl	17.18783149	-2.62678278	0.55082399
Cl	14.95342717	-3.70721497	-1.34347236
Cl	12.84072112	-5.12947173	0.44954034
Cl	7.79941975	6.21530842	0.95613680
Cl	5.64993340	5.01588677	-0.93940049
Cl	3.53146686	3.75465984	0.95458219
Cl	1.38807208	2.55192000	-0.94474458
Cl	19.16474467	-1.29809789	-1.45625999
C	8.54410177	-0.02031412	-0.12549667
O	15.78649434	-0.51045084	2.46858686
H	16.63969082	-0.88105704	2.75097307

H	15.06269429	-1.32625881	2.55666369
O	14.19924789	-2.42137916	2.50188405
H	13.33310404	-2.00578064	2.69989232
H	14.32101079	-2.77933535	1.25601166

**f. Transition State 5**

C	2.17042645	1.19195855	-0.20758716
C	4.28936242	-0.02254013	-0.06190971
C	6.42007245	-1.25835520	-0.09226611
C	8.54998698	-2.49411225	-0.23563594
C	10.68683784	-3.73895790	-0.36452300
C	4.30519074	2.41570155	0.17321404
C	6.41898014	1.20922946	-0.06971102
C	9.97155756	-0.02797998	-0.13625459
C	10.68435199	-1.26643653	-0.20690778
C	12.82005005	-2.51761635	-0.32160746
C	6.43155748	3.65263949	-0.20655967
C	8.55098221	2.43776133	-0.06514696
C	10.68306581	1.20253554	-0.10375377
C	12.81775535	-0.03657653	-0.23147812
C	14.95698534	-1.28109394	-0.29395450
C	8.56792206	4.87531048	0.17297113
C	10.68179964	3.66893466	-0.07111846
C	12.81403456	2.43206952	-0.11010243
C	14.94893711	1.19097937	-0.15526751
C	17.08283366	-0.04922594	-0.32062397
C	3.57179798	1.22350092	-0.02934971
C	5.70813146	-0.01994540	-0.05854721
C	7.83839247	-1.25621757	-0.14330355
C	9.96921733	-2.49214947	-0.27052724
C	12.08724428	-3.71972678	-0.20125289
C	5.70102913	2.45581190	-0.03613029
C	7.83737090	1.21133475	-0.09981021
C	12.10336271	-1.26567353	-0.25995113

C	14.22696336	-2.47537771	-0.50361277
C	7.83331663	3.68383281	-0.03010826
C	9.97039335	2.44033691	-0.06355281
C	12.10298518	1.20232377	-0.14400328
C	14.23782534	-0.03584413	-0.22975848
C	16.36176629	-1.25127605	-0.15488984
C	9.96335070	4.91537730	-0.03766146
C	12.10019227	3.67041182	-0.09671716
C	14.23537956	2.42811218	-0.10633802
C	16.36462099	1.19558504	-0.23322799
C	18.46905207	-0.00435110	-0.58177894
Cl	17.18315873	-2.63548011	0.49946155
Cl	14.99449074	-3.78235907	-1.35325124
Cl	12.87263008	-5.12748791	0.45052929
Cl	7.79841644	6.21183976	0.95832210
Cl	5.64955825	5.01403234	-0.93705009
Cl	3.53373203	3.75310336	0.95522154
Cl	1.38786591	2.55206013	-0.93996190
Cl	19.20212463	-1.30731902	-1.46159497
C	8.55073870	-0.02663472	-0.12198060
O	15.84220895	-0.47496408	2.47415692
H	16.67466905	-0.88838978	2.74286163
H	15.17910535	-1.20389379	2.57111717
O	14.01555308	-2.44285747	2.64082596
H	13.17498898	-2.01190529	2.85897913
H	13.94603531	-2.68456296	1.69258094

**g. Final**

C	2.17512786	1.17780796	-0.22704158
C	4.29591690	-0.03733098	-0.07139037
C	6.42808525	-1.27241833	-0.08912815
C	8.55915535	-2.50590905	-0.24278093
C	10.69277412	-3.74090871	-0.43780915
C	4.30938755	2.40127298	0.14832139

C	6.42540125	1.19296518	-0.07734572
C	9.97925864	-0.04165333	-0.11140140
C	10.69287635	-1.27675996	-0.19438311
C	12.82631708	-2.50922962	-0.43762405
C	6.43626976	3.63787127	-0.22722548
C	8.55716327	2.42279813	-0.07176929
C	10.68975709	1.18930387	-0.08959722
C	12.82372592	-0.04264753	-0.24381460
C	14.95659628	-1.28019026	-0.44219454
C	8.57113318	4.86135131	0.14753186
C	10.68765109	3.65376298	-0.07742942
C	12.82098556	2.42032024	-0.10768965
C	14.95615070	1.18147514	-0.19393381
C	17.08798165	-0.05126206	-0.44068433
C	3.57637140	1.20876707	-0.04946943
C	5.71460407	-0.03523689	-0.06009741
C	7.84743986	-1.27072428	-0.13041274
C	9.97782921	-2.50095715	-0.28176363
C	12.10130794	-3.71810331	-0.33246561
C	5.70646292	2.43987997	-0.05739087
C	7.84365699	1.19705076	-0.09882753
C	12.11029935	-1.26867839	-0.27984677
C	14.21644288	-2.45835980	-0.70031039
C	7.83795035	3.66901483	-0.05016930
C	9.97600258	2.42605029	-0.06058597
C	12.10977682	1.19143788	-0.13188265
C	14.24210960	-0.04120903	-0.28259573
C	16.36441022	-1.25910267	-0.34006197
C	9.96815591	4.90023271	-0.05764061
C	12.10602489	3.65716177	-0.09920712
C	14.24255701	2.41620399	-0.11151632
C	16.37201537	1.18677301	-0.27863273
C	18.47688413	0.00158219	-0.69742182



Cl	17.18111987	-2.68014892	0.22649722
Cl	14.93571637	-3.72340285	-1.64297411
Cl	12.92466056	-5.13194186	0.26153756
Cl	7.79564886	6.20372877	0.92062677
Cl	5.65242680	4.99646869	-0.96829552
Cl	3.53412523	3.74328406	0.92299706
Cl	1.39162377	2.53613310	-0.96928247
Cl	19.21674518	-1.25772581	-1.63209369
C	8.55796922	-0.04034464	-0.10685611
O	15.89518130	-0.45691362	2.63523858
H	16.71445270	-0.89187928	2.90869064
H	15.20861256	-1.15236491	2.72737844
O	13.75627629	-2.32539988	2.85421260
H	12.96663746	-1.92722268	3.24961487
H	13.45280681	-2.74116589	2.02992142

## 5) HOOH formation

### a. Initial

C	2.20361563	1.21039728	-0.23507235
C	4.32298370	0.00132233	-0.06873285
C	6.45631196	-1.22715722	-0.08419186
C	8.58583295	-2.45994439	-0.19019568
C	10.70815793	-3.71848646	-0.35659995
C	4.33777438	2.43596013	0.16290179
C	6.45140350	1.23436719	-0.07135286
C	9.99988940	-0.00114398	-0.15160056
C	10.70974520	-1.23760444	-0.23027665
C	12.82316795	-2.47493993	-0.25712854
C	6.46245687	3.67483248	-0.22371038
C	8.58187238	2.46397064	-0.07092763
C	10.71231460	1.22777243	-0.11691610
C	12.83751602	-0.00357861	-0.22402114
C	14.94467925	-1.21401510	-0.01250830
C	8.60228324	4.89679028	0.16353398

C	10.71490266	3.69004984	-0.07659442
C	12.84566495	2.45924518	-0.10742514
C	14.98325741	1.23544910	-0.04618177
C	17.12723619	0.00074465	-0.10152254
C	3.60442148	1.24501981	-0.04670709
C	5.74254827	0.00553788	-0.05814275
C	7.87389075	-1.22831667	-0.13650429
C	10.00497416	-2.47170949	-0.26062901
C	12.12476727	-3.68046638	-0.22178622
C	5.73396501	2.47780443	-0.04232400
C	7.86969216	1.23618759	-0.10253896
C	12.12692259	-1.23689765	-0.27050611
C	14.29546501	-2.48851537	-0.25129398
C	7.86381078	3.70936636	-0.04170477
C	10.00186457	2.46275501	-0.06736462
C	12.13590935	1.22428564	-0.15404554
C	14.26676749	-0.00928303	-0.11077224
C	16.34374367	-1.13841570	0.50576746
C	9.99855405	4.93339318	-0.04811806
C	12.13601839	3.68973043	-0.10278529
C	14.27276895	2.45693506	-0.08029619
C	16.40810407	1.23638642	-0.07961704
C	18.46019261	0.00131693	-0.49274804
Cl	17.19074747	-2.74709756	0.59523107
Cl	14.89200049	-3.12204632	-1.99571610
Cl	13.01944981	-5.12483290	0.13268077
Cl	7.83523899	6.23971662	0.94508819
Cl	5.67752225	5.03530489	-0.95364050
Cl	3.55791314	3.77296849	0.94259200
Cl	1.42070604	2.56398047	-0.97941888
Cl	19.12580721	-1.35185259	-1.34035817
C	8.58062928	0.00287049	-0.12611954
O	16.05133697	-0.77344925	1.88004477

O	17.29133905	-0.40058024	2.64210322
H	17.59427619	-1.29591520	2.89946033
H	14.17760660	-1.23499954	3.40219554
O	13.42638852	-1.78400545	3.12766721
H	12.75437367	-1.66310268	3.81191955
H	14.70104361	-3.27884127	0.38979748

**b. Transition State 1**

C	2.19957930	1.21952369	-0.22698673
C	4.31908744	0.01087994	-0.06108582
C	6.45327995	-1.21918680	-0.08633877
C	8.58344822	-2.45608002	-0.20617166
C	10.70798052	-3.70285546	-0.38839250
C	4.33460164	2.44644239	0.16620564
C	6.44849140	1.24221232	-0.06458732
C	9.99779924	0.00870727	-0.13501661
C	10.70804427	-1.22658206	-0.21803696
C	12.81361186	-2.46304766	-0.29907188
C	6.45960958	3.68238332	-0.22420676
C	8.57961623	2.47123612	-0.06461549
C	10.71204089	1.23580667	-0.10443664
C	12.84361909	0.00489103	-0.25197509
C	14.98557228	-1.19919655	-0.22405758
C	8.59822787	4.90515309	0.16582869
C	10.71230898	3.69894180	-0.06910035
C	12.84523690	2.46731668	-0.11207290
C	14.98188041	1.24126915	-0.15270697
C	17.11687074	-0.00297933	-0.27110091
C	3.59984006	1.25618159	-0.03847610
C	5.73890482	0.01430412	-0.05118378
C	7.87146864	-1.22242034	-0.13192419
C	10.00132269	-2.46068307	-0.25966097
C	12.12673772	-3.66614524	-0.26232648
C	5.73074185	2.48585950	-0.03963772

C	7.86691330	1.24366479	-0.09465865
C	12.12238543	-1.22572021	-0.28498278
C	14.28216191	-2.48180636	-0.32834434
C	7.86086901	3.71729777	-0.03929393
C	9.99995346	2.47083359	-0.05986631
C	12.13615482	1.23256567	-0.15328924
C	14.27383181	0.01328720	-0.24986932
C	16.37349273	-1.20232611	-0.04186012
C	9.99499244	4.94217800	-0.04166647
C	12.13205435	3.70096718	-0.09655676
C	14.26703880	2.47030834	-0.10835590
C	16.40222803	1.23701228	-0.18084725
C	18.48251438	0.03293058	-0.59635491
Cl	17.19592265	-2.68575782	0.31902694
Cl	14.89536383	-3.21982665	-1.94313390
Cl	13.01389209	-5.10994083	0.10205850
Cl	7.82827908	6.24579295	0.94669017
Cl	5.67600839	5.04130365	-0.95687113
Cl	3.55898062	3.78563948	0.94416660
Cl	1.41570197	2.57452887	-0.96512009
Cl	19.17583716	-1.25454281	-1.52472076
C	8.57836360	0.00878192	-0.11283670
O	15.95440347	-0.80454270	2.23778113
O	17.17430953	-0.46972770	2.82986647
H	17.53298484	-1.34282864	3.09418937
H	14.51138186	-1.64432187	2.90426571
O	13.66861910	-2.14558923	2.99923228
H	13.00525690	-1.45270739	3.14125997
H	14.66076972	-3.18091730	0.42606477

**c. Transition State 2**

C	2.19228149	1.21831619	-0.22473105
C	4.31181130	0.01009137	-0.05834651
C	6.44542965	-1.21834810	-0.08829508

C	8.57471615	-2.45293859	-0.22566703
C	10.69982773	-3.69927012	-0.41980014
C	4.32748396	2.44595858	0.16552994
C	6.44094469	1.24164092	-0.06235306
C	9.98938410	0.01009931	-0.14523504
C	10.69781585	-1.22333200	-0.25452398
C	12.79767112	-2.45449168	-0.41340235
C	6.45226919	3.68096488	-0.22191527
C	8.57210057	2.47027241	-0.06205182
C	10.70335152	1.23641704	-0.10937483
C	12.83297176	0.01199290	-0.29379362
C	14.97417181	-1.18922082	-0.28408429
C	8.59081886	4.90487631	0.16477543
C	10.70441276	3.69864142	-0.06715564
C	12.83649987	2.46800945	-0.11407059
C	14.97186205	1.24649756	-0.18558024
C	17.10667970	0.00662322	-0.30521300
C	3.59253620	1.25547457	-0.03705883
C	5.73164293	0.01455810	-0.04914376
C	7.86320836	-1.22097860	-0.13664794
C	9.99249125	-2.45874359	-0.28126975
C	12.12083823	-3.65958428	-0.32859482
C	5.72322930	2.48539192	-0.03896916
C	7.85889725	1.24336860	-0.09156670
C	12.11015569	-1.21643343	-0.36800113
C	14.26885881	-2.47509735	-0.40539470
C	7.85342851	3.71641532	-0.03782828
C	9.99222579	2.47096606	-0.05837240
C	12.12598870	1.23537421	-0.16631985
C	14.26142576	0.02311807	-0.29140821
C	16.35312241	-1.18623156	-0.09710317
C	9.98709432	4.94217113	-0.04105687
C	12.12379505	3.70148635	-0.09384111

C	14.25740163	2.47354358	-0.11862796
C	16.39118894	1.24313220	-0.22349158
C	18.47595692	0.03511484	-0.61116520
Cl	17.14773211	-2.64921028	0.37460918
Cl	14.89872716	-3.31760698	-1.89055169
Cl	13.00376464	-5.08599368	0.09926842
Cl	7.81927698	6.24623185	0.94431588
Cl	5.66766816	5.04022890	-0.95500096
Cl	3.55063101	3.78439547	0.94466212
Cl	1.40787754	2.57421087	-0.96424261
Cl	19.17132270	-1.27908012	-1.50220648
C	8.57037434	0.00889356	-0.11211872
O	15.88999256	-0.46905198	2.24910068
O	17.16078159	-0.47546597	2.82630024
H	17.28478170	-1.41508948	3.09244290
H	14.70214619	-1.66346480	2.56100848
O	13.92270022	-2.27531616	2.62839256
H	13.15815729	-1.68592700	2.69180492
H	14.57263696	-3.10248921	0.44392241

**d. Transition State 3**

C	2.18933981	1.21468559	-0.22200204
C	4.30850857	0.00512816	-0.05755807
C	6.44079041	-1.22470062	-0.08548345
C	8.56922436	-2.46099998	-0.22467419
C	10.69690882	-3.70420620	-0.42284043
C	4.32458005	2.44186379	0.16563928
C	6.43735064	1.23712237	-0.06194835
C	9.98379398	0.00398292	-0.13617253
C	10.68996014	-1.22979043	-0.24736753
C	12.78649941	-2.45586877	-0.47054492
C	6.44940513	3.67695001	-0.21936933
C	8.56846879	2.46537339	-0.06071018
C	10.69819353	1.23109953	-0.10383106

C	12.82549404	0.00752347	-0.30636700
C	14.97119822	-1.18857824	-0.41138265
C	8.58795229	4.90077849	0.16511117
C	10.70100488	3.69439439	-0.06608159
C	12.83232522	2.46273132	-0.11201179
C	14.96699195	1.23940929	-0.20392659
C	17.10541228	-0.00102979	-0.35122105
C	3.58973368	1.25077994	-0.03574595
C	5.72813595	0.00951343	-0.04833294
C	7.85838884	-1.22751441	-0.13164537
C	9.98638227	-2.46531157	-0.27983488
C	12.11653173	-3.66356053	-0.34649133
C	5.72007990	2.48104682	-0.03845249
C	7.85486442	1.23842920	-0.09027206
C	12.09917672	-1.22132861	-0.38081653
C	14.25555570	-2.46838834	-0.48244507
C	7.85062115	3.71174115	-0.03628587
C	9.98838320	2.46645510	-0.05646889
C	12.12030903	1.23127955	-0.16145359
C	14.25219588	0.02251848	-0.33592874
C	16.34998687	-1.20073818	-0.20922767
C	9.98413590	4.93825842	-0.04044590
C	12.12008436	3.69687078	-0.09215111
C	14.25324798	2.46686891	-0.11780223
C	16.38641615	1.23379127	-0.24156674
C	18.47960866	0.02963919	-0.62624649
Cl	17.12633671	-2.65895211	0.31179911
Cl	14.90209050	-3.41538730	-1.83796949
Cl	13.00223811	-5.07693505	0.12023632
Cl	7.81657522	6.24246856	0.94449761
Cl	5.66558341	5.03607573	-0.95364959
Cl	3.54794886	3.78057332	0.94433653
Cl	1.40550539	2.57045773	-0.96225937

Cl	19.19177218	-1.27906312	-1.51434304
C	8.56546766	0.00301270	-0.10766701
O	15.84237497	-0.45732281	2.25386053
O	17.11833897	-0.50288117	2.82957366
H	17.23270072	-1.44823173	3.07571181
H	14.89345315	-1.61050760	2.38187515
O	14.17838522	-2.35033455	2.28524050
H	13.32171604	-1.90367354	2.32306442
H	14.42073018	-2.83382974	0.62110866

**e. Transition State 4**

C	2.18940645	1.21450167	-0.22005624
C	4.30853094	0.00460996	-0.05681605
C	6.44076286	-1.22738735	-0.08621297
C	8.56988305	-2.46415636	-0.22478357
C	10.69979067	-3.70809322	-0.42386689
C	4.32447562	2.44213644	0.16517395
C	6.43788216	1.23597420	-0.06164658
C	9.98523142	0.00191085	-0.13537515
C	10.69442940	-1.23358055	-0.23847010
C	12.80524553	-2.46473169	-0.46254727
C	6.44944019	3.67669932	-0.21734707
C	8.56873461	2.46486041	-0.06011388
C	10.69926391	1.23058446	-0.10404622
C	12.82924289	0.00457731	-0.29503822
C	14.96256307	-1.22106595	-0.41381342
C	8.58782233	4.90116339	0.16445861
C	10.70141895	3.69390049	-0.06550538
C	12.83203804	2.46158879	-0.11251314
C	14.96623009	1.23075133	-0.19850535
C	17.10278166	-0.01021469	-0.35254212
C	3.59032150	1.24991267	-0.03502034
C	5.72816305	0.00826596	-0.04939422
C	7.85885561	-1.22910910	-0.13113070



C	9.98767645	-2.46636453	-0.28032352
C	12.11296858	-3.67494257	-0.35081300
C	5.72076741	2.47976367	-0.03754794
C	7.85538423	1.23794222	-0.09039274
C	12.10824993	-1.22259203	-0.35075294
C	14.24225260	-2.46167933	-0.55949543
C	7.85119986	3.71070789	-0.03560748
C	9.98838661	2.46672316	-0.05670726
C	12.11911872	1.23310912	-0.16205827
C	14.24971733	0.01155096	-0.31520504
C	16.35474985	-1.21083992	-0.22109370
C	9.98445769	4.93765666	-0.03987514
C	12.11965152	3.69723036	-0.09149034
C	14.25331793	2.46325171	-0.11766940
C	16.38585606	1.22930225	-0.24247748
C	18.48080214	0.02519270	-0.62556709
Cl	17.13018397	-2.66599632	0.31274743
Cl	14.90545384	-3.51316763	-1.78538729
Cl	12.99965830	-5.08548930	0.12648181
Cl	7.81583747	6.24356445	0.94458676
Cl	5.66536137	5.03622044	-0.95389464
Cl	3.54764207	3.78179194	0.94480809
Cl	1.40533468	2.57099011	-0.96225924
Cl	19.19244403	-1.28146201	-1.51699878
C	8.56644911	0.00134335	-0.10806574
O	15.74621657	-0.53016223	2.26830033
O	17.07767320	-0.52503294	2.83326115
H	17.23753057	-1.45984414	3.07176615
H	15.06522026	-1.49945983	2.38015195
O	14.19363922	-2.41743232	2.13430855
H	13.33900504	-1.94766090	2.24538642
H	14.31659005	-2.69138713	0.99049503

**f. Transition State 5**

C	2.18927602	1.20212577	-0.21941473
C	4.30858766	-0.01172186	-0.06290148
C	6.43971159	-1.24882693	-0.08832071
C	8.56842766	-2.48784498	-0.23669686
C	10.70117513	-3.73053140	-0.42830740
C	4.32571187	2.42630610	0.16456544
C	6.43904102	1.21876128	-0.06819966
C	9.98778677	-0.02006070	-0.11680087
C	10.69836915	-1.25915496	-0.19657818
C	12.82741504	-2.49273095	-0.41952969
C	6.45005603	3.66243961	-0.21583393
C	8.56916264	2.44818888	-0.06481204
C	10.69958913	1.21256083	-0.09361647
C	12.82994795	-0.02133221	-0.24101358
C	14.96045627	-1.26146953	-0.41692151
C	8.58777547	4.88656864	0.16357468
C	10.70089937	3.67925291	-0.07020443
C	12.83098319	2.44351270	-0.10657426
C	14.96371239	1.20196254	-0.19074605
C	17.09464695	-0.03765393	-0.42903303
C	3.58983333	1.23563410	-0.03755469
C	5.72802331	-0.00974407	-0.05475326
C	7.85873098	-1.24969843	-0.13030913
C	9.98683170	-2.48731385	-0.27544493
C	12.11083124	-3.70529297	-0.33221012
C	5.72152234	2.46553811	-0.04116432
C	7.85628676	1.22071616	-0.09437037
C	12.11599649	-1.24994825	-0.27520481
C	14.22894950	-2.45497032	-0.63654579
C	7.85111535	3.69587978	-0.03770222
C	9.98838801	2.45133059	-0.05870974
C	12.11897017	1.21497292	-0.13685630
C	14.24801366	-0.02156622	-0.27343108

C	16.36797644	-1.24534100	-0.32990746
C	9.98324858	4.92598477	-0.04368405
C	12.11862610	3.68172023	-0.09412940
C	14.25209228	2.43924149	-0.11144019
C	16.37987046	1.20430880	-0.27138321
C	18.48385733	0.00975261	-0.67648592
Cl	17.16487098	-2.68143798	0.23283830
Cl	14.90881718	-3.61094796	-1.73280509
Cl	12.96856844	-5.11694778	0.19750622
Cl	7.81612375	6.22866700	0.94359760
Cl	5.66565526	5.02402532	-0.94823641
Cl	3.55061566	3.76654446	0.94469191
Cl	1.40619092	2.56175513	-0.95690773
Cl	19.21867566	-1.26836701	-1.58754581
C	8.56792450	-0.01839931	-0.10686118
O	15.78963890	-0.55751855	2.27730183
O	17.06096021	-0.50342838	3.03371238
H	17.43469037	-1.39111601	2.86310177
H	15.22512601	-1.20611456	2.77012819
O	13.79309115	-2.32480547	2.66876409
H	12.99476413	-1.77349294	2.71283774
H	13.90344509	-2.50778811	1.71483201

**g. Final**

C	2.18490372	1.19400900	-0.22171259
C	4.30501656	-0.02099813	-0.06716259
C	6.43638887	-1.25775283	-0.08812125
C	8.56557172	-2.49346168	-0.23773929
C	10.69718354	-3.72988235	-0.43490912
C	4.32085310	2.41709655	0.15826970
C	6.43509453	1.20985779	-0.07321036
C	9.98650385	-0.02717994	-0.10842113
C	10.69804841	-1.26446494	-0.18711835
C	12.82960728	-2.49738172	-0.43464934

C	6.44603847	3.65387556	-0.22121381
C	8.56624301	2.43934533	-0.06764512
C	10.69831191	1.20464687	-0.08843662
C	12.83015922	-0.02960992	-0.24034445
C	14.96144925	-1.27274654	-0.45681148
C	8.58267843	4.87751034	0.15693611
C	10.69754321	3.67073669	-0.07367184
C	12.82895397	2.43483797	-0.10481437
C	14.96266166	1.19161039	-0.19028962
C	17.09378402	-0.04289141	-0.44806936
C	3.58586332	1.22585002	-0.04286816
C	5.72424712	-0.01884988	-0.05806068
C	7.85559644	-1.25672306	-0.12882232
C	9.98347499	-2.48950693	-0.27603402
C	12.10568705	-3.70774550	-0.33044337
C	5.71692723	2.45664241	-0.04847415
C	7.85288072	1.21240245	-0.09598406
C	12.11577363	-1.25617519	-0.27400487
C	14.21564640	-2.44826131	-0.71359616
C	7.84717488	3.68603894	-0.04306408
C	9.98583682	2.44269971	-0.05879258
C	12.11825211	1.20576414	-0.13011082
C	14.24838721	-0.03232541	-0.28172810
C	16.37123505	-1.25416225	-0.37171117
C	9.97866269	4.91731713	-0.04949329
C	12.11531193	3.67283094	-0.09584141
C	14.25003999	2.42944588	-0.10906021
C	16.37931684	1.19710047	-0.27532995
C	18.48262633	0.01368466	-0.70495854
Cl	17.19933397	-2.69398798	0.12082010
Cl	14.91218052	-3.70872829	-1.68022288
Cl	12.93022413	-5.12352190	0.25111139
Cl	7.80832069	6.21942369	0.93534945

Cl	5.66162560	5.01427162	-0.95764387
Cl	3.54690760	3.75814675	0.93783924
Cl	1.40117610	2.55472756	-0.95836947
Cl	19.22949815	-1.22271343	-1.66484069
C	8.56568846	-0.02574377	-0.10439423
O	15.95455188	-0.84803909	2.42040109
O	17.15642345	-0.45982942	3.18785993
H	17.49860932	-1.34341033	3.42071057
H	15.24123152	-0.81762185	3.09589814
O	13.50544361	-1.70675670	3.20743916
H	12.62741976	-1.73502884	3.61281363
H	13.42433600	-2.21948260	2.38600087

## 6) OO Dissociation

### a. Initial

C	2.15353540	1.20107393	-0.15148771
C	4.27573488	-0.01579542	-0.05678407
C	6.40648835	-1.24591021	-0.09270146
C	8.53745260	-2.47553649	-0.12160613
C	10.66263803	-3.72507298	-0.09532626
C	4.29092324	2.41842253	0.22427859
C	6.40436530	1.21922599	-0.06254698
C	9.96045031	-0.01761642	-0.09770800
C	10.67294292	-1.25581260	-0.08465589
C	12.76738395	-2.51659226	0.08934397
C	6.41572525	3.66134182	-0.16274275
C	8.54037437	2.44681034	-0.06243755
C	10.67394712	1.20875520	-0.08939558
C	12.81218522	-0.03990140	-0.10103286
C	14.97471547	-1.24429995	0.08538144
C	8.55199984	4.87772867	0.22605012
C	10.66793344	3.67746884	-0.05938127
C	12.80306610	2.43770987	-0.10322769
C	14.93677953	1.20266017	-0.08385415

C	17.07966285	-0.02230327	-0.09768062
C	3.55750566	1.22812011	0.00430654
C	5.69458806	-0.01039803	-0.06152306
C	7.82513757	-1.24065463	-0.11552715
C	9.95477598	-2.48116706	-0.09064306
C	12.05721367	-3.70377898	0.18473500
C	5.68526750	2.46320455	-0.00356659
C	7.82427263	1.22201094	-0.09966371
C	12.09027497	-1.27121479	-0.07439075
C	14.24819101	-2.53662729	0.25443217
C	7.82067891	3.68958476	-0.00253426
C	9.96018368	2.44659469	-0.06326040
C	12.09973188	1.19707183	-0.10201307
C	14.23839487	-0.03208193	-0.07594209
C	16.35890066	-1.22144613	0.17371034
C	9.94812626	4.92135689	0.00417096
C	12.08743724	3.67664336	-0.09688085
C	14.22155536	2.44012823	-0.09626160
C	16.35739957	1.21382457	-0.08882929
C	18.46819579	0.00651430	-0.33001198
Cl	17.24576524	-2.55109291	0.84471782
Cl	14.94616630	-3.75353475	-0.90697058
Cl	12.76234157	-5.13348229	0.86582244
Cl	7.79160063	6.18825728	1.06900153
Cl	5.61886659	5.04663557	-0.83698850
Cl	3.53451749	3.73267742	1.06605859
Cl	1.35340747	2.58637388	-0.82143097
Cl	19.23568443	-1.31428041	-1.14700216
C	8.53807682	-0.01317516	-0.10941908
O	14.51785557	-3.01464144	1.69344084
O	14.05644985	-2.06650051	2.51343352

**b. Transition State 1**

C	2.15346281	1.20175144	-0.14779559
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C	4.27601251	-0.01535295	-0.05670259
C	6.40710489	-1.24541958	-0.09162957
C	8.53848711	-2.47365121	-0.12024383
C	10.66410621	-3.72333506	-0.11797956
C	4.29164942	2.41873465	0.22636072
C	6.40504858	1.21982407	-0.06276112
C	9.96136386	-0.01760371	-0.09790955
C	10.67412534	-1.25591977	-0.08968111
C	12.76833395	-2.51773071	0.06005161
C	6.41640170	3.66169468	-0.16208045
C	8.54116810	2.44668905	-0.06294153
C	10.67513257	1.20833266	-0.09002245
C	12.81267691	-0.04167855	-0.10074517
C	14.97886290	-1.24603219	0.07612917
C	8.55222938	4.87756616	0.22839832
C	10.66832686	3.67765419	-0.05977734
C	12.80355996	2.43772835	-0.10198591
C	14.93748246	1.20291803	-0.07897254
C	17.08086717	-0.01888191	-0.10930903
C	3.55788640	1.22886602	0.00580111
C	5.69492037	-0.00986112	-0.06171267
C	7.82589290	-1.23968092	-0.11385399
C	9.95551617	-2.48053193	-0.09464421
C	12.06177751	-3.70745629	0.13440774
C	5.68572573	2.46355649	-0.00324568
C	7.82495715	1.22221497	-0.09972369
C	12.09029551	-1.27205144	-0.08452547
C	14.25071888	-2.54182121	0.22789085
C	7.82134904	3.68949184	-0.00226893
C	9.96104544	2.44645834	-0.06380677
C	12.10086284	1.19624030	-0.10069070
C	14.23994563	-0.03371348	-0.07243801
C	16.36435571	-1.21996082	0.15832060

C	9.94831680	4.92167229	0.00561906
C	12.08792577	3.67675902	-0.09682932
C	14.22238993	2.44053576	-0.09356429
C	16.35809764	1.21613202	-0.08798658
C	18.46512047	0.01372094	-0.36765102
Cl	17.25748415	-2.56093557	0.79890573
Cl	14.95199607	-3.73308277	-0.95691303
Cl	12.77356678	-5.15849558	0.76086722
Cl	7.79133694	6.18624087	1.07469477
Cl	5.61943124	5.04802186	-0.83445271
Cl	3.53743030	3.73265793	1.07055657
Cl	1.35163922	2.59016479	-0.80921891
Cl	19.20001786	-1.28229452	-1.24981831
C	8.53914749	-0.01273968	-0.10893480
O	14.48762363	-3.00521575	1.66914734
O	13.56783118	-2.36421189	2.39757597

**c. Transition State 2**

C	2.15350634	1.20450021	-0.14056482
C	4.27713849	-0.01250690	-0.05363343
C	6.40856570	-1.24212333	-0.09103972
C	8.54273591	-2.46829931	-0.12814507
C	10.67222739	-3.71952460	-0.12936433
C	4.29244096	2.42140712	0.23071901
C	6.40617009	1.22330842	-0.06112877
C	9.96183637	-0.01404577	-0.10594891
C	10.67312516	-1.25181115	-0.08967050
C	12.76063269	-2.50514661	0.16340585
C	6.41641276	3.66440271	-0.16105965
C	8.54176968	2.44935213	-0.06295312
C	10.67716470	1.21173144	-0.09343687
C	12.81344039	-0.04088046	-0.09438389
C	14.99017200	-1.23479641	0.07857181
C	8.55248020	4.87906476	0.23185966



C	10.66903915	3.68040303	-0.05718472
C	12.80510563	2.44074215	-0.10446450
C	14.94026752	1.20850879	-0.08052194
C	17.08473600	-0.00923990	-0.12442687
C	3.55859464	1.23125472	0.01142361
C	5.69622419	-0.00686556	-0.05984043
C	7.82831384	-1.23590580	-0.11533630
C	9.95670269	-2.47657278	-0.09985406
C	12.05746893	-3.71765732	0.15096454
C	5.68658772	2.46612919	-0.00101522
C	7.82566861	1.22539406	-0.10084211
C	12.08672633	-1.26586625	-0.06981215
C	14.26727064	-2.53164952	0.25823709
C	7.82165179	3.69141539	-0.00140013
C	9.96231710	2.44927740	-0.06407729
C	12.10233818	1.19930906	-0.10499255
C	14.24437287	-0.02972429	-0.06993800
C	16.37513348	-1.20959244	0.15030871
C	9.94919937	4.92384787	0.01098227
C	12.08926131	3.67942367	-0.09605229
C	14.22354824	2.44538160	-0.09376839
C	16.35907025	1.22188513	-0.09480257
C	18.46534325	0.02586687	-0.40421732
Cl	17.25702739	-2.56135821	0.78264248
Cl	14.91365558	-3.71032910	-0.97692679
Cl	12.76396225	-5.18436172	0.74812225
Cl	7.79099163	6.18598795	1.07843671
Cl	5.61952912	5.05035404	-0.83309730
Cl	3.53893481	3.73502920	1.07445013
Cl	1.35155285	2.59268867	-0.80246325
Cl	19.18480324	-1.26436875	-1.30243998
C	8.53995985	-0.00913801	-0.11279143
O	14.41815309	-2.94163947	1.66291812

O 13.23365839 -2.36916534 2.15487641

**d. Transition State 3**

C 2.15402642 1.20469083 -0.14050991  
C 4.27744754 -0.01278150 -0.05360787  
C 6.40946293 -1.24295554 -0.09050676  
C 8.55062754 -2.46766944 -0.12925261  
C 10.68456044 -3.72173421 -0.13629555  
C 4.29243996 2.42116658 0.23051786  
C 6.40696060 1.22339467 -0.06124638  
C 9.96325029 -0.01363118 -0.11082595  
C 10.67867577 -1.24965817 -0.08313467  
C 12.78281983 -2.48725208 0.37726915  
C 6.41614587 3.66433857 -0.16097493  
C 8.54214452 2.44949790 -0.06310740  
C 10.67864538 1.21208387 -0.09452900  
C 12.81088032 -0.04329684 -0.08911410  
C 14.99639336 -1.23409602 0.07908916  
C 8.55284897 4.87908826 0.23229533  
C 10.66922945 3.67987877 -0.05739663  
C 12.80657875 2.44149359 -0.10692557  
C 14.94265721 1.20648785 -0.08185953  
C 17.08589585 -0.00893456 -0.12307713  
C 3.55828018 1.23126454 0.01141850  
C 5.69675469 -0.00725890 -0.05989417  
C 7.83049498 -1.23543749 -0.11447957  
C 9.95820731 -2.47496667 -0.10243402  
C 12.04723903 -3.73817116 0.17904958  
C 5.68662768 2.46666144 -0.00083909  
C 7.82553715 1.22560959 -0.10152229  
C 12.08684830 -1.25336434 -0.02864394  
C 14.30385417 -2.54723478 0.27374199  
C 7.82177777 3.69170612 -0.00147649  
C 9.96219032 2.45065359 -0.06334463

C	12.10166973	1.20109288	-0.11033506
C	14.24979344	-0.03334493	-0.06642668
C	16.38104066	-1.20592438	0.14978592
C	9.94877148	4.92379065	0.00989619
C	12.08993442	3.67957156	-0.09632454
C	14.22422551	2.44537292	-0.09447189
C	16.36053198	1.21914350	-0.09813220
C	18.46866522	0.02353129	-0.41091185
Cl	17.25908219	-2.56175514	0.78072987
Cl	14.89335603	-3.70413826	-0.99609295
Cl	12.75576671	-5.19627587	0.75835792
Cl	7.79076233	6.18656406	1.07836476
Cl	5.61935215	5.05062972	-0.83289074
Cl	3.53881114	3.73507914	1.07446403
Cl	1.35150378	2.59260957	-0.80371853
Cl	19.18281717	-1.26479630	-1.30966897
C	8.54018546	-0.00981557	-0.11488833
O	14.47300626	-2.99027266	1.64045341
O	13.12878703	-2.39556200	1.98045730

**e. Transition State 4**

C	2.15441960	1.20560883	-0.14007692
C	4.27947920	-0.01111006	-0.05349691
C	6.41401924	-1.24115560	-0.09129273
C	8.56050701	-2.46519170	-0.12918527
C	10.69273157	-3.72481226	-0.12756611
C	4.29351955	2.42233574	0.23089212
C	6.40882801	1.22429395	-0.06135685
C	9.96931039	-0.01216198	-0.11200542
C	10.69072611	-1.24457116	-0.07821199
C	12.80969353	-2.47625612	0.45616791
C	6.41697068	3.66508346	-0.16099845
C	8.54387646	2.45120447	-0.06296847
C	10.68332533	1.21571556	-0.09618986

C	12.81957589	-0.03793205	-0.08593134
C	15.01118025	-1.23432100	0.09037281
C	8.55334758	4.88065299	0.23310883
C	10.67057219	3.68217468	-0.05633390
C	12.80951503	2.44457216	-0.10839769
C	14.95145962	1.20853919	-0.08705045
C	17.09486108	-0.00758932	-0.13078283
C	3.55958779	1.23265753	0.01236925
C	5.69902161	-0.00602998	-0.06039003
C	7.83635360	-1.23345059	-0.11532392
C	9.97060378	-2.47329653	-0.09717476
C	12.06189334	-3.74494835	0.22488974
C	5.68790331	2.46710258	-0.00086115
C	7.82808471	1.22669298	-0.10248639
C	12.10060956	-1.24259514	-0.02203426
C	14.33083417	-2.53808831	0.37619060
C	7.82279306	3.69262011	-0.00114346
C	9.96453134	2.45298036	-0.06368204
C	12.10505975	1.20685965	-0.11123432
C	14.26119835	-0.03386053	-0.06594143
C	16.39369834	-1.20641316	0.14743251
C	9.94949917	4.92544394	0.01277536
C	12.09184214	3.68172170	-0.09616374
C	14.22937016	2.44727219	-0.09723559
C	16.37026727	1.22397143	-0.10168716
C	18.47729330	0.02526873	-0.41091746
Cl	17.26773676	-2.56420393	0.76067876
Cl	14.84902247	-3.68410849	-1.08773056
Cl	12.77201097	-5.19587357	0.76047803
Cl	7.79036474	6.18741339	1.07848940
Cl	5.62024354	5.05052545	-0.83274060
Cl	3.54015971	3.73607391	1.07410448
Cl	1.35276671	2.59314098	-0.80287859

Cl	19.18569629	-1.26116470	-1.30759199
C	8.54469232	-0.00808509	-0.11635543
O	14.63464964	-2.98306260	1.61797239
O	12.68157038	-2.47401485	1.87388921

**f. Transition State 5**

C	2.14913182	1.22194416	-0.10300810
C	4.27537762	0.00406879	-0.04194626
C	6.41146919	-1.22352026	-0.09290518
C	8.54701992	-2.45640905	-0.13440658
C	10.65113156	-3.73587602	-0.12654898
C	4.29501827	2.43653328	0.24862294
C	6.40687964	1.23531693	-0.05770122
C	9.96859687	-0.00728248	-0.11247999
C	10.69137170	-1.24097916	-0.08933965
C	12.80347497	-2.47713792	0.26852239
C	6.41489958	3.67545138	-0.15891287
C	8.54187008	2.46109068	-0.05997317
C	10.67715679	1.22316316	-0.10095460
C	12.81695246	-0.01481049	-0.12083144
C	15.01108388	-1.18605103	0.07272965
C	8.54822376	4.88910180	0.24914380
C	10.66548517	3.69420586	-0.04563828
C	12.80160021	2.46099643	-0.10485205
C	14.93834926	1.23830512	-0.07889261
C	17.07781052	0.01629360	-0.22425498
C	3.55690644	1.24720253	0.03722385
C	5.69640290	0.00812187	-0.05740221
C	7.83114161	-1.22298782	-0.11492469
C	9.96409920	-2.48363471	-0.08005307
C	12.04619498	-3.76519820	0.35800486
C	5.68688989	2.47679846	0.00594254
C	7.82768367	1.23391682	-0.09929790
C	12.10174913	-1.22739703	-0.09253505

C	14.31588250	-2.46148807	0.36909753
C	7.82111826	3.70191886	0.00418510
C	9.96097346	2.46205846	-0.06123244
C	12.09864859	1.22288260	-0.12218366
C	14.25385650	0.00445068	-0.06459535
C	16.41267845	-1.18031521	0.11153359
C	9.94567261	4.93683324	0.03574758
C	12.08616704	3.69619652	-0.08842688
C	14.22169210	2.46880522	-0.09272906
C	16.35962849	1.24269585	-0.12776181
C	18.46831373	0.04892526	-0.48898995
Cl	17.34569894	-2.49687225	0.70895003
Cl	14.98171076	-3.74165104	-0.97323970
Cl	12.82491605	-5.33598132	0.60189739
Cl	7.77718887	6.18786464	1.09785996
Cl	5.62130437	5.05814725	-0.83758019
Cl	3.55451678	3.75600216	1.09367312
Cl	1.34352127	2.61479689	-0.74913216
Cl	19.19052534	-1.22274130	-1.39972071
C	8.54304951	0.00054116	-0.11020773
O	14.69749494	-2.51702352	1.62349180
O	12.20743760	-2.97300364	1.50444105

**g. Final**

C	2.14896814	1.22112289	-0.10344698
C	4.27578348	0.00357921	-0.04439086
C	6.41132658	-1.22330096	-0.08958892
C	8.54717701	-2.45387740	-0.13760210
C	10.65522082	-3.73206804	-0.14704778
C	4.29400227	2.43554256	0.25095760
C	6.40681175	1.23537763	-0.05772733
C	9.96873127	-0.00687005	-0.11147548
C	10.69071433	-1.24033942	-0.08347192
C	12.80645954	-2.46738637	0.32189161

C	6.41455126	3.67578494	-0.15367920
C	8.54161373	2.46055242	-0.06013605
C	10.67791215	1.22356442	-0.09980437
C	12.81675804	-0.01341659	-0.12286873
C	15.00509466	-1.18816635	0.04572239
C	8.54845950	4.88925389	0.25045390
C	10.66599056	3.69357411	-0.04752185
C	12.80103417	2.46014927	-0.10310274
C	14.94011265	1.24197562	-0.09115243
C	17.07283649	0.01728671	-0.24290639
C	3.55670648	1.24743912	0.03596191
C	5.69636355	0.00824223	-0.05592276
C	7.83173019	-1.22313032	-0.11429980
C	9.96594246	-2.48137108	-0.08366468
C	12.04809043	-3.76485284	0.35903626
C	5.68604489	2.47752097	0.00878358
C	7.82797913	1.23387419	-0.10038936
C	12.10580965	-1.22809266	-0.07983763
C	14.30442645	-2.38792943	0.54919227
C	7.82026860	3.70279113	0.00657489
C	9.96122366	2.46128048	-0.06181424
C	12.09870018	1.22358625	-0.12006542
C	14.25541641	0.00443978	-0.09066468
C	16.39862247	-1.17989261	0.07739860
C	9.94510957	4.93727481	0.03522204
C	12.08632114	3.69544053	-0.09017994
C	14.22215018	2.46964296	-0.08838940
C	16.35907199	1.24598884	-0.13426545
C	18.46428404	0.05661274	-0.51566270
Cl	17.30062711	-2.52560974	0.62653416
Cl	14.81586446	-3.45397893	-1.52138363
Cl	12.90216738	-5.29115775	0.53198205
Cl	7.78013189	6.18821163	1.09521329

Cl	5.62120476	5.05617754	-0.83234512
Cl	3.55171474	3.75032888	1.09436738
Cl	1.34623438	2.61082453	-0.75447670
Cl	19.19111786	-1.20244351	-1.42771708
C	8.54429648	0.00131885	-0.11160229
O	14.71597478	-2.78133387	1.66579012
O	12.13770918	-2.98359913	1.51655532

### ER Mechanism – ZU Bromine

#### 1) OOH formation

##### a. Initial

C	2.16253138	1.17479297	-0.20719883
C	4.28032119	-0.03914097	-0.07166800
C	6.41037947	-1.27275372	-0.08524636
C	8.54329187	-2.51324118	-0.09669132
C	10.67578627	-3.76103278	-0.07515153
C	4.29637302	2.39636371	0.18636325
C	6.40864032	1.19383142	-0.07582069
C	9.96172655	-0.04640242	-0.08562993
C	10.67346055	-1.28412612	-0.06929093
C	12.78127036	-2.53481427	0.01597721
C	6.42357116	3.63686556	-0.20462946
C	8.54282707	2.42243251	-0.07193872
C	10.67344396	1.18293851	-0.08596305
C	12.80823383	-0.06269810	-0.11074524
C	14.95536673	-1.27747504	0.02476588
C	8.55985006	4.85648432	0.18409298
C	10.67211477	3.65101875	-0.07867551
C	12.80513210	2.41388682	-0.10315230
C	14.93762598	1.17716020	-0.06757527
C	17.07660138	-0.06615839	-0.07153342
C	3.56250848	1.20818680	-0.02964572
C	5.69850940	-0.03570766	-0.06519947
C	7.83106252	-1.27491620	-0.10064821



C	9.96157568	-2.51333128	-0.06728772
C	12.08120788	-3.71996809	0.13696532
C	5.68996972	2.44138504	-0.03538953
C	7.82766092	1.19658270	-0.10481908
C	12.08745112	-1.29325763	-0.08668808
C	14.24340089	-2.55662326	-0.09651236
C	7.82468180	3.66947163	-0.03025849
C	9.96157754	2.42139214	-0.06714168
C	12.09816343	1.17409588	-0.10079725
C	14.23346678	-0.05195518	-0.08553779
C	16.33407685	-1.25961162	0.15058077
C	9.95374003	4.89848753	-0.03856101
C	12.09152361	3.65303891	-0.10781077
C	14.22502804	2.41440059	-0.08562893
C	16.35719727	1.17813858	-0.06555511
C	18.46554713	-0.02196619	-0.31976491
Br	17.21891359	-2.83534061	0.78323748
Br	14.61939453	-3.18434880	-2.06817984
Br	13.01017495	-5.27725774	0.74665797
Br	7.75008458	6.26698537	1.18996816
Br	5.58271859	5.09535535	-1.11553059
Br	3.48238922	3.80531175	1.19153085
Br	1.32237542	2.63169642	-1.12126984
Br	19.23970534	-1.37840164	-1.42340534
C	8.54015459	-0.04141273	-0.10154772
O	16.15931748	0.20864356	3.28683732
O	15.77883055	-0.42420103	4.29058375
H	14.08744953	-1.46100865	3.60347282
O	13.32210996	-1.82931761	3.13161166
H	12.60183051	-1.78998914	3.77922061
H	14.70844134	-3.36584111	0.46056246

**b. Transition State 1**

C	2.14353887	1.17308990	-0.19524089
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C	4.25880363	-0.04023226	-0.06615298
C	6.38675980	-1.27515391	-0.08941643
C	8.51712698	-2.51355426	-0.11612029
C	10.64613659	-3.76151213	-0.07609201
C	4.27662604	2.39375465	0.20236885
C	6.38716285	1.19168716	-0.06873441
C	9.93899613	-0.04863104	-0.09341658
C	10.64895164	-1.28758389	-0.08341908
C	12.75557637	-2.54053001	0.05804160
C	6.40496572	3.63514924	-0.19324785
C	8.52171405	2.42128487	-0.06678499
C	10.65092636	1.18016795	-0.08816754
C	12.78709771	-0.06670755	-0.11438715
C	14.93640920	-1.27968807	0.06745781
C	8.53973114	4.85372071	0.20177375
C	10.65074887	3.64888464	-0.07101991
C	12.78323665	2.41130035	-0.10356721
C	14.91497442	1.17357219	-0.08099275
C	17.05308813	-0.06513843	-0.07832532
C	3.54303494	1.20715817	-0.01932915
C	5.67610682	-0.03805064	-0.06237154
C	7.80647454	-1.27556969	-0.11144466
C	9.93457105	-2.51519146	-0.08443275
C	12.04195306	-3.72098063	0.19451131
C	5.67015028	2.43973920	-0.02181949
C	7.80671505	1.19516440	-0.10137679
C	12.06581824	-1.29996295	-0.09251831
C	14.22966304	-2.57702549	0.11583418
C	7.80549844	3.66831494	-0.01952838
C	9.93990272	2.41888124	-0.06444867
C	12.07612704	1.17064630	-0.10512739
C	14.21391617	-0.05954737	-0.09034557
C	16.31621474	-1.25354169	0.19697813

C	9.93353274	4.89695555	-0.02367837
C	12.07050562	3.65116025	-0.10340578
C	14.20252599	2.41109703	-0.09279652
C	16.33350101	1.17698893	-0.08256098
C	18.44293526	-0.02886261	-0.30539333
Br	17.20641299	-2.74145585	1.00028593
Br	14.87139450	-3.66856585	-1.52473674
Br	12.88241099	-5.23621768	0.99102672
Br	7.73204999	6.25828021	1.21663314
Br	5.56136193	5.09899759	-1.09061825
Br	3.46545569	3.79648635	1.21742163
Br	1.29990421	2.63571761	-1.09457054
Br	19.25396979	-1.44184738	-1.30466638
C	8.51797229	-0.04309156	-0.10498972
O	16.21468477	-0.07841968	2.76467710
O	15.70527637	-0.63400611	3.75790817
H	14.22853917	-1.66576203	3.24754074
O	13.53772241	-2.30703443	3.00289107
H	12.84881911	-1.78744331	2.56675047
H	14.55616731	-3.16972203	0.97576678

**c. Transition State 2**

C	2.14110114	1.17656033	-0.19449615
C	4.25607462	-0.03625375	-0.06427866
C	6.38346912	-1.27104104	-0.08650332
C	8.51297587	-2.50797630	-0.12062973
C	10.63918004	-3.75384204	-0.09874699
C	4.27407723	2.39669675	0.20418191
C	6.38424166	1.19560171	-0.06714854
C	9.93469162	-0.04280038	-0.08927239
C	10.64287447	-1.28129086	-0.08863157
C	12.75104551	-2.53820322	-0.05424185
C	6.40250776	3.63850326	-0.19240621
C	8.51857206	2.42499797	-0.06488254

C	10.64793715	1.18520049	-0.08595333
C	12.78430111	-0.06063467	-0.12509708
C	14.93699684	-1.28147087	-0.01252087
C	8.53716471	4.85642378	0.20407153
C	10.64804709	3.65323261	-0.06882706
C	12.78027199	2.41620803	-0.10023767
C	14.91263267	1.17931826	-0.08367577
C	17.04976597	-0.05771216	-0.09244266
C	3.54045525	1.21050021	-0.01800283
C	5.67305068	-0.03423914	-0.06061284
C	7.80311070	-1.27066986	-0.10914006
C	9.92963178	-2.50922910	-0.09459176
C	12.03717344	-3.71482235	0.13589901
C	5.66757880	2.44327667	-0.02043552
C	7.80363400	1.19911394	-0.09940661
C	12.05846810	-1.29312812	-0.12250495
C	14.20816960	-2.55097938	0.12326287
C	7.80255008	3.67140288	-0.01802942
C	9.93689901	2.42313511	-0.06274904
C	12.07307497	1.17663725	-0.10278791
C	14.21254025	-0.05406944	-0.11059622
C	16.31481036	-1.24910537	0.16687786
C	9.93088246	4.90075698	-0.02180383
C	12.06780975	3.65536645	-0.10105798
C	14.19948077	2.41561710	-0.08907425
C	16.33068720	1.18296044	-0.09144827
C	18.43886186	-0.02371636	-0.31512614
Br	17.19485474	-2.67801076	1.08076921
Br	15.01390766	-3.90262987	-1.15219916
Br	12.83380322	-5.19955041	1.03998602
Br	7.72979950	6.26094478	1.21977783
Br	5.55899286	5.10333674	-1.08810115
Br	3.46320770	3.79969926	1.21972326

Br	1.29651385	2.63922340	-1.09292306
Br	19.25104984	-1.44871637	-1.29496928
C	8.51450702	-0.03834761	-0.10116424
O	15.94525376	-0.02633450	2.60831788
O	15.58810181	-0.73672104	3.58852506
H	14.48103361	-1.65109374	3.09117470
O	13.79082963	-2.34201466	2.80069866
H	12.96218995	-1.88484836	2.58367641
H	14.20639967	-2.72747025	1.34119468

**d. Transition State 3**

C	2.14040434	1.17656502	-0.19433312
C	4.25571537	-0.03627474	-0.06431470
C	6.38381667	-1.27241104	-0.08669888
C	8.51464729	-2.51060525	-0.12138506
C	10.64826320	-3.75467211	-0.09862563
C	4.27349638	2.39680344	0.20419191
C	6.38436184	1.19484802	-0.06736180
C	9.93555714	-0.04307350	-0.08828809
C	10.64614849	-1.28234618	-0.07951697
C	12.77395981	-2.53738575	-0.06489401
C	6.40190840	3.63825836	-0.19200351
C	8.51812880	2.42478284	-0.06477599
C	10.64870513	1.18596783	-0.08635542
C	12.78583900	-0.05927271	-0.11790084
C	14.92881942	-1.29634888	-0.02941668
C	8.53672873	4.85663574	0.20426133
C	10.64768047	3.65297740	-0.06882950
C	12.77954145	2.41629385	-0.10088565
C	14.91331411	1.17756742	-0.07381955
C	17.04860855	-0.06326978	-0.09109733
C	3.53962877	1.21098167	-0.01807625
C	5.67264889	-0.03447907	-0.06151743
C	7.80366144	-1.27167796	-0.10777399

C	9.93273834	-2.50818677	-0.09642248
C	12.04094831	-3.72592649	0.12518368
C	5.66701427	2.44348729	-0.02012237
C	7.80345705	1.19912372	-0.09989684
C	12.06438578	-1.28652108	-0.10008834
C	14.20012351	-2.51429191	-0.12398574
C	7.80171981	3.67173071	-0.01780707
C	9.93603835	2.42428448	-0.06274293
C	12.07065249	1.18174511	-0.10606692
C	14.20644945	-0.05310490	-0.08838428
C	16.32614801	-1.25306418	0.15924444
C	9.92975594	4.90170472	-0.02188289
C	12.06666216	3.65634824	-0.10046904
C	14.19969970	2.41493810	-0.08742447
C	16.32920739	1.18156032	-0.09263381
C	18.44122858	-0.02549998	-0.31129953
Br	17.19302397	-2.67864306	1.08374184
Br	15.02908244	-3.92596366	-1.14817890
Br	12.83644764	-5.20339384	1.04016449
Br	7.72867005	6.26121932	1.21939497
Br	5.55865051	5.10396790	-1.08736934
Br	3.46284131	3.80000275	1.21946908
Br	1.29566129	2.63967277	-1.09229101
Br	19.25119785	-1.44893730	-1.29765468
C	8.51552025	-0.03959103	-0.10159190
O	15.92887562	-0.04818457	2.60155518
O	15.49210719	-0.85789317	3.57867538
H	14.70630640	-1.50062630	3.14284717
O	13.78292231	-2.39193025	2.64811710
H	12.94385231	-1.91260449	2.54586308
H	14.05063805	-2.61857057	1.69054281

**e. Transition State 4**

C	2.16007748	1.17920913	-0.19606708
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C	4.27858914	-0.03545353	-0.06714371
C	6.41001052	-1.27293314	-0.08250865
C	8.54339335	-2.51408740	-0.11640931
C	10.67952988	-3.76006675	-0.14179711
C	4.29488096	2.39896203	0.19797203
C	6.40685988	1.19514830	-0.07251221
C	9.96291243	-0.04578637	-0.08086020
C	10.67731404	-1.28606401	-0.07709798
C	12.81480527	-2.53796803	-0.14585000
C	6.42106228	3.63939853	-0.19511766
C	8.54011624	2.42495660	-0.06724654
C	10.67164970	1.18722840	-0.08211013
C	12.80645147	-0.05495706	-0.12021218
C	14.94481543	-1.29701360	-0.10159051
C	8.55743135	4.85915915	0.19580357
C	10.66939717	3.65499181	-0.07321498
C	12.80265564	2.41871498	-0.09832002
C	14.93655330	1.17653095	-0.07269125
C	17.07157139	-0.06787339	-0.10730830
C	3.56043789	1.21223033	-0.02162466
C	5.69615903	-0.03421279	-0.06333613
C	7.83127349	-1.27444295	-0.09811514
C	9.96207052	-2.51222859	-0.10638502
C	12.07995482	-3.73305332	0.03807928
C	5.68793709	2.44421497	-0.02692275
C	7.82615125	1.19840626	-0.10167209
C	12.09578207	-1.28479917	-0.11316413
C	14.22060319	-2.49526056	-0.31124095
C	7.82151557	3.67281927	-0.02229578
C	9.95801082	2.42630961	-0.06316197
C	12.09310513	1.18545124	-0.10040180
C	14.22578785	-0.05093993	-0.10066647
C	16.34787917	-1.26336503	0.07875364

C	9.95005659	4.90436029	-0.02940119
C	12.08818961	3.65821656	-0.10180907
C	14.22414848	2.41472097	-0.08196722
C	16.35499703	1.17890288	-0.09743491
C	18.46398912	-0.02867614	-0.33537018
Br	17.21892997	-2.79017553	0.80392994
Br	15.05709398	-3.95375467	-1.24948223
Br	12.88039276	-5.17743255	1.00975391
Br	7.74891627	6.26462940	1.21062097
Br	5.57628350	5.10472129	-1.09090258
Br	3.48622899	3.80171079	1.21599583
Br	1.31710724	2.64455956	-1.09375615
Br	19.27294369	-1.45747908	-1.31661236
C	8.54099194	-0.04126167	-0.09745538
O	15.97803962	-0.02877427	2.60419827
O	15.61757712	-0.87404539	3.58349635
H	14.77175976	-1.33083439	3.26474369
O	13.42510637	-2.15297149	2.90063365
H	12.56944403	-1.80788556	3.05865840
H	13.47826954	-2.46229612	1.94597195

**f. Transition State 5**

C	2.17474991	1.17224544	-0.20903628
C	4.29531557	-0.04502504	-0.07662992
C	6.43219694	-1.28257798	-0.07967308
C	8.56996898	-2.52392757	-0.11736568
C	10.70977636	-3.75875450	-0.23333260
C	4.31416382	2.39167317	0.17689766
C	6.42349649	1.18523095	-0.07991174
C	9.98416680	-0.05122430	-0.07815719
C	10.69569785	-1.29115903	-0.06956055
C	12.84061526	-2.53075449	-0.17761856
C	6.44174708	3.63366430	-0.21298566
C	8.55524518	2.41534375	-0.07504622



C	10.69350545	1.18076665	-0.07971755
C	12.82735604	-0.06146575	-0.11176045
C	14.97280516	-1.30783650	-0.16958125
C	8.57268417	4.85173854	0.17814205
C	10.68710298	3.64600815	-0.08110217
C	12.82725416	2.41022680	-0.09763516
C	14.95945627	1.16283638	-0.07418752
C	17.10107531	-0.08264902	-0.15581924
C	3.57307176	1.20229728	-0.03653614
C	5.71645105	-0.04338944	-0.06611058
C	7.85152204	-1.28508864	-0.09445810
C	9.99442932	-2.51591012	-0.15246979
C	12.10837244	-3.72750013	0.00041363
C	5.70770320	2.43380259	-0.04688634
C	7.84586232	1.18901881	-0.10879455
C	12.11840357	-1.28592509	-0.12650184
C	14.23151754	-2.49322789	-0.38219762
C	7.84044870	3.66302816	-0.03798934
C	9.97476880	2.41732556	-0.06579160
C	12.11309278	1.17737173	-0.09447392
C	14.24549077	-0.06404527	-0.10988590
C	16.36984591	-1.27849546	0.01698182
C	9.96594161	4.89502949	-0.04530357
C	12.10360375	3.64757817	-0.10785880
C	14.24998913	2.40423841	-0.07827063
C	16.38268896	1.16646359	-0.10210345
C	18.49492222	-0.03089452	-0.37539337
Br	17.21804477	-2.77805881	0.83004331
Br	15.00573960	-3.90327067	-1.41855562
Br	12.94545557	-5.19215236	0.92289783
Br	7.77222204	6.25884117	1.18924017
Br	5.69777674	5.09014189	-1.22620101
Br	3.56294549	3.92149868	1.03226153

Br	1.41653506	2.61895065	-1.21845523
Br	19.33093426	-1.42262708	-1.38064880
C	8.55856476	-0.05097380	-0.09729540
O	16.43095790	-0.39331494	2.82584062
O	15.09509275	-0.56577505	3.03588933
H	14.98465225	-1.60515219	3.06373884
O	13.18714175	-2.36425044	3.17597695
H	12.68623363	-1.54039020	3.24274483
H	13.01041816	-2.69461537	2.27259583

**g. Final**

C	2.21572277	1.21795569	-0.23335760
C	4.33572872	0.00854439	-0.06743055
C	6.47065315	-1.22748865	-0.08197599
C	8.60250279	-2.46231772	-0.19692999
C	10.73642085	-3.70690202	-0.42869448
C	4.35152144	2.44162531	0.16728954
C	6.46677376	1.23679172	-0.07054856
C	10.01918361	0.00208240	-0.12781237
C	10.73305793	-1.23617470	-0.22733635
C	12.87445826	-2.46343415	-0.42985268
C	6.47613617	3.67905114	-0.23066429
C	8.59559653	2.47024455	-0.06882582
C	10.72738539	1.23446124	-0.10067511
C	12.86110575	0.00083967	-0.18660088
C	14.97726656	-1.25761520	-0.10345660
C	8.61326460	4.90288261	0.16744075
C	10.72894755	3.69758436	-0.07160157
C	12.86048195	2.46334737	-0.09645581
C	14.99538888	1.22252522	-0.01885274
C	17.15823599	-0.00478437	-0.12441400
C	3.61578506	1.25496933	-0.04609493
C	5.75568556	0.00884506	-0.05660962
C	7.88918984	-1.22614803	-0.13212159

C	10.02349935	-2.46563594	-0.29072923
C	12.15037086	-3.67681995	-0.34542544
C	5.74722967	2.48302573	-0.04333015
C	7.88533126	1.24175532	-0.09982377
C	12.15234435	-1.23041427	-0.28603228
C	14.30980835	-2.39010336	-0.53604141
C	7.87550755	3.71724937	-0.04381110
C	10.01484206	2.47093069	-0.06130187
C	12.14890034	1.23598138	-0.12896378
C	14.27001143	-0.00980413	-0.06700749
C	16.37265064	-1.15454546	0.46664014
C	10.00928640	4.94349875	-0.04490067
C	12.14764082	3.70073889	-0.09776578
C	14.28529750	2.45570155	-0.07176259
C	16.42681403	1.23325261	-0.07904355
C	18.48384407	0.00504793	-0.52735327
Br	17.31945024	-2.90126533	0.80782852
Br	15.21318274	-3.67126020	-1.63382318
Br	13.04823423	-5.20155249	0.38374405
Br	7.79519536	6.32538411	1.15063529
Br	5.64013539	5.12595454	-1.16178936
Br	3.52998621	3.86151670	1.15111169
Br	1.38113317	2.66412529	-1.16745050
Br	19.15590991	-1.45056848	-1.56824314
C	8.59902692	0.00503212	-0.11589717
O	16.26978001	-0.63047532	1.82994494
O	15.17581240	-1.26526037	2.56834060
H	15.62045298	-2.07201818	2.90590709
O	12.57084593	-2.30479997	3.36060194
H	11.68666802	-1.92172121	3.44216194
H	13.04156605	-1.71115950	2.75073189

**2) O formation**  
**a. Initial**

C	2.21888548	1.22243686	-0.24810243
C	4.33726879	0.01726033	-0.06874983
C	6.47089698	-1.21321735	-0.08418910
C	8.60092300	-2.44609260	-0.20178980
C	10.72344354	-3.70061647	-0.42141481
C	4.35305157	2.44782857	0.16654405
C	6.46658300	1.24855362	-0.07237951
C	10.01633926	0.01364098	-0.14534025
C	10.72710138	-1.22271692	-0.22910453
C	12.84840794	-2.46460821	-0.27422175
C	6.47855665	3.68739960	-0.24401409
C	8.59683552	2.47990025	-0.07213928
C	10.72698155	1.24227198	-0.11108908
C	12.85386888	0.00675069	-0.20584739
C	14.95120521	-1.21450700	0.00801642
C	8.61636588	4.90824243	0.16774439
C	10.72983590	3.70465947	-0.07521278
C	12.86047894	2.47286846	-0.10408378
C	14.99410036	1.24687021	-0.03909489
C	17.13629137	0.01410943	-0.14530147
C	3.61741658	1.26227365	-0.05026112
C	5.75684170	0.01956942	-0.05634124
C	7.88923901	-1.21389155	-0.13890301
C	10.02020628	-2.45521967	-0.27772041
C	12.13976133	-3.67166146	-0.29353556
C	5.74749120	2.49382904	-0.04881609
C	7.88568728	1.25177462	-0.10380062
C	12.14323549	-1.22497956	-0.26667913
C	14.30347801	-2.44883127	-0.26936752
C	7.87684329	3.72631967	-0.04887427
C	10.01633058	2.47736895	-0.06410492
C	12.15025169	1.23767584	-0.14527693
C	14.27791010	0.00421776	-0.09005843

C	16.36000502	-1.11555691	0.48771801
C	10.01140263	4.94964324	-0.04967354
C	12.15064751	3.70585813	-0.10278263
C	14.28608770	2.47149092	-0.07805530
C	16.41928692	1.25165734	-0.09022386
C	18.45751701	0.02861530	-0.58086590
Br	17.28221213	-2.91859800	0.60457834
Br	14.88605626	-2.83942713	-2.46690080
Br	13.11649564	-5.26786501	0.08815852
Br	7.80133969	6.33338469	1.14482562
Br	5.64542333	5.13168666	-1.17520294
Br	3.52757159	3.86861903	1.14094297
Br	1.38796371	2.65939490	-1.19140179
Br	19.07468728	-1.37095379	-1.71295576
C	8.59734968	0.01787230	-0.12482297
O	16.37328570	-0.60981722	1.85176175
O	15.48292943	-1.44352919	2.68367409
H	16.01475396	-2.26968052	2.74213597
H	13.61362011	-1.57090173	3.23204622
O	12.81768289	-2.12615569	3.30370449
H	12.41435813	-1.87438387	4.14678481
H	14.79267276	-3.34603246	0.09615740

**b. Transition State 1**

C	2.21541001	1.22202022	-0.23841616
C	4.33412982	0.01834364	-0.06097426
C	6.46866017	-1.21029030	-0.08712061
C	8.59615738	-2.44382476	-0.21310238
C	10.71834428	-3.69056206	-0.43384725
C	4.34775718	2.45147163	0.17032969
C	6.46185443	1.25055121	-0.06601836
C	10.01149295	0.01745939	-0.13538081
C	10.72219547	-1.21855045	-0.22084843
C	12.83072073	-2.46097683	-0.29236603

C	6.47369449	3.69003606	-0.23388427
C	8.59185268	2.48225915	-0.06296105
C	10.72170207	1.24463397	-0.10554116
C	12.84947676	0.01034091	-0.23131625
C	14.96253135	-1.20262472	-0.09578523
C	8.61152121	4.91155850	0.17447077
C	10.72602621	3.70503072	-0.06620144
C	12.85693738	2.47286111	-0.11012013
C	14.99379121	1.25047266	-0.09406140
C	17.14209361	0.01620609	-0.21579998
C	3.61481620	1.26224068	-0.04011428
C	5.75352566	0.02172095	-0.05143394
C	7.88493567	-1.21180444	-0.13989440
C	10.01817128	-2.45039934	-0.28088448
C	12.13180023	-3.66906177	-0.29234951
C	5.74322845	2.49437048	-0.04133369
C	7.88109385	1.25428104	-0.09772613
C	12.13407444	-1.22425164	-0.27461449
C	14.28852446	-2.45169456	-0.31340755
C	7.87262371	3.72775108	-0.03864490
C	10.01133632	2.47878921	-0.05697815
C	12.14411941	1.24119034	-0.15193037
C	14.26831360	0.01614674	-0.16316612
C	16.35594425	-1.11525062	0.43834639
C	10.00810209	4.94837086	-0.03837307
C	12.14663381	3.70703698	-0.09713403
C	14.28506736	2.47390062	-0.09824374
C	16.42348436	1.25242377	-0.12748233
C	18.45541891	0.04393866	-0.63541396
Br	17.31258862	-3.00509153	0.50774067
Br	14.90781769	-2.96551421	-2.35972751
Br	13.10325936	-5.26050237	0.08849560
Br	7.79846093	6.33784632	1.14989585

Br	5.64349947	5.13084694	-1.17291366
Br	3.52062603	3.87201397	1.14265596
Br	1.38729236	2.65152931	-1.19455123
Br	19.09432777	-1.33952459	-1.78040250
C	8.59323384	0.02076727	-0.11793203
O	16.17352102	-0.71280060	1.68953138
O	15.53310803	-1.77559979	3.57171560
H	16.03653092	-2.47135626	3.09438475
H	13.78688231	-1.82074050	3.40533351
O	12.80979511	-1.93017473	3.27861104
H	12.43821002	-1.87471957	4.16832290
H	14.76355579	-3.28753198	0.20960832

**c. Transition State 2**

C	2.21422052	1.22487177	-0.23685787
C	4.33279921	0.02002793	-0.06025406
C	6.46932268	-1.20799072	-0.08616242
C	8.59874736	-2.44789188	-0.20139894
C	10.72054259	-3.68817267	-0.43707593
C	4.34728604	2.45353851	0.16803488
C	6.46192317	1.25179768	-0.06561931
C	10.01138638	0.02020793	-0.13335055
C	10.72366359	-1.21576193	-0.21864459
C	12.82005988	-2.45751480	-0.30577943
C	6.47345158	3.69154266	-0.23294046
C	8.59247162	2.48271874	-0.06301886
C	10.72268826	1.24602921	-0.10467006
C	12.85738933	0.01692088	-0.24452656
C	14.96842399	-1.20049119	-0.08332349
C	8.61088899	4.91301269	0.17195209
C	10.72654207	3.70741225	-0.06538430
C	12.85840605	2.47523763	-0.11319569
C	14.99300540	1.25193324	-0.10828236
C	17.15829511	0.01313303	-0.20860999

C	3.61300162	1.26504712	-0.04080920
C	5.75300529	0.02433282	-0.05089182
C	7.88498039	-1.21138693	-0.13660170
C	10.01921269	-2.44955213	-0.27634603
C	12.13155272	-3.66621995	-0.30190572
C	5.74247091	2.49686269	-0.04198153
C	7.88066800	1.25522785	-0.09691272
C	12.13244605	-1.22026217	-0.28054197
C	14.27357091	-2.45455784	-0.35744759
C	7.87228110	3.72919557	-0.03932593
C	10.01138316	2.48095619	-0.05663838
C	12.14597149	1.24582460	-0.15564812
C	14.26862118	0.03765816	-0.20166309
C	16.39225037	-1.16159491	0.32724561
C	10.00746070	4.95152778	-0.03924035
C	12.14529957	3.71143682	-0.09627291
C	14.28287719	2.47993761	-0.10371270
C	16.42950195	1.24702418	-0.11901449
C	18.46979759	0.04639516	-0.63381531
Br	17.33352591	-2.98179637	0.49460506
Br	14.92957912	-3.09160129	-2.25255421
Br	13.10323876	-5.26003421	0.09262629
Br	7.79712398	6.33943198	1.14906270
Br	5.64257204	5.13348806	-1.17178304
Br	3.51966734	3.87438909	1.14179537
Br	1.38615405	2.65370212	-1.19548312
Br	19.10891997	-1.33361823	-1.78839225
C	8.59316552	0.02022010	-0.11695306
O	15.84797242	-0.88253886	1.53219846
O	15.57404398	-1.79418586	3.60477933
H	16.03729068	-2.49430497	3.09739439
H	13.79935134	-1.83101345	3.42089696
O	12.82708634	-1.92018803	3.28308773



H	12.44330005	-1.86340458	4.16768661
H	14.72652928	-3.26881550	0.23026543

**d. Transition State 3**

C	2.20719856	1.23379955	-0.23992079
C	4.32512137	0.02793374	-0.05950274
C	6.45985955	-1.20211297	-0.08108016
C	8.58939147	-2.44738743	-0.17454203
C	10.71218075	-3.68181725	-0.43341315
C	4.34082253	2.46203259	0.16328324
C	6.45617909	1.25781747	-0.06324326
C	10.00452293	0.02753288	-0.14034568
C	10.71575844	-1.20709935	-0.24427621
C	12.80397765	-2.44639362	-0.36972521
C	6.46719005	3.69776470	-0.23820559
C	8.58660636	2.48796243	-0.06288474
C	10.71645915	1.25384544	-0.11705805
C	12.84775161	0.03100683	-0.31492776
C	14.94844236	-1.20018922	-0.05033956
C	8.60323178	4.92130246	0.16177405
C	10.71892419	3.71657395	-0.07102629
C	12.84918262	2.48382710	-0.12834112
C	14.97745047	1.25703836	-0.14022089
C	17.14894247	0.01138033	-0.19558922
C	3.60511918	1.27415847	-0.04457416
C	5.74566046	0.03129141	-0.04650452
C	7.87670300	-1.20822267	-0.11940034
C	10.00757669	-2.44233756	-0.26961895
C	12.12405655	-3.65789676	-0.32938792
C	5.73624007	2.50406803	-0.04629277
C	7.87426245	1.26000941	-0.09395553
C	12.12200068	-1.20851483	-0.34611428
C	14.25861736	-2.45742113	-0.40148763
C	7.86556513	3.73541330	-0.04467841

C	10.00505671	2.48871490	-0.05954819
C	12.13700848	1.25721482	-0.19024483
C	14.25092899	0.06052551	-0.26790008
C	16.40922823	-1.21112653	0.20405342
C	9.99982787	4.96081977	-0.04923512
C	12.13674151	3.72115385	-0.09888037
C	14.26941158	2.49077702	-0.11712158
C	16.41749765	1.24422803	-0.10248507
C	18.46042618	0.05706841	-0.62734492
Br	17.36904350	-2.94792265	0.46716590
Br	14.95134054	-3.21768837	-2.14538091
Br	13.10091525	-5.24661300	0.09219515
Br	7.79110761	6.34149662	1.15330180
Br	5.63555852	5.13976935	-1.17568937
Br	3.51818039	3.88428983	1.13889365
Br	1.37625418	2.66872839	-1.18940899
Br	19.11270286	-1.32446849	-1.77679064
C	8.58655515	0.02295367	-0.11029074
O	15.57714674	-1.05503355	1.30310265
O	15.59443837	-1.75109791	3.91390297
H	16.05554030	-2.31574197	3.25356628
H	13.94544011	-1.86813960	3.27079632
O	13.09691253	-1.94126230	2.77815078
H	12.48445034	-2.25943710	3.46921681
H	14.68815308	-3.24861855	0.22524694

**e. Transition State 4**

C	2.19873183	1.24510504	-0.24934453
C	4.31489348	0.03411165	-0.06058115
C	6.44814700	-1.19778098	-0.07797717
C	8.57499579	-2.44187696	-0.17217882
C	10.68615236	-3.66959007	-0.46459744
C	4.33185074	2.47129768	0.15260895
C	6.44564052	1.26482175	-0.06654021

C	9.99278777	0.03425115	-0.15117511
C	10.69881732	-1.19918998	-0.27079218
C	12.77917815	-2.44104073	-0.46776429
C	6.45929603	3.70454787	-0.24767591
C	8.57662393	2.49414603	-0.06555704
C	10.70613248	1.26103725	-0.13215655
C	12.83580637	0.03453863	-0.36536238
C	14.93516140	-1.20215825	-0.08525021
C	8.59418763	4.93084130	0.14796759
C	10.70805738	3.72512170	-0.07738292
C	12.83790701	2.48774214	-0.14312188
C	14.96596845	1.25859229	-0.15056359
C	17.13629696	0.01846268	-0.20688057
C	3.59590273	1.28213486	-0.05055121
C	5.73543456	0.03732711	-0.04610577
C	7.86422492	-1.20297313	-0.11328577
C	9.99066644	-2.43469018	-0.28135555
C	12.09700523	-3.64747318	-0.38626160
C	5.72652156	2.51208761	-0.05707825
C	7.86403146	1.26539255	-0.09378437
C	12.10177743	-1.20253300	-0.41976776
C	14.24366381	-2.46028441	-0.44552767
C	7.85704584	3.74259727	-0.05340528
C	9.99580222	2.49575944	-0.06394787
C	12.12528551	1.26171509	-0.22389029
C	14.24067663	0.06482493	-0.31053152
C	16.40630559	-1.20981728	0.17435281
C	9.98918790	4.97230287	-0.06223058
C	12.12618385	3.72669974	-0.10274870
C	14.25869892	2.49424445	-0.12177194
C	16.40540506	1.24827232	-0.10587599
C	18.44397695	0.06915984	-0.65762311
Br	17.41587178	-2.89348360	0.43387022

Br	14.97310197	-3.34377545	-2.03820761
Br	13.02379750	-5.22633279	0.16017310
Br	7.77543979	6.35418306	1.12508319
Br	5.62763277	5.14540133	-1.18723949
Br	3.51105111	3.89347308	1.13043802
Br	1.36971218	2.68687214	-1.18956600
Br	19.09045176	-1.25036421	-1.88270341
C	8.57488106	0.02831385	-0.10776956
O	15.55304564	-1.07934891	1.27445482
O	15.28890583	-1.82388801	3.91327784
H	16.00238574	-2.09136037	3.31218258
H	14.52176155	-1.76936335	3.28311273
O	13.38880586	-2.27336188	2.26092484
H	12.73290824	-2.64630435	2.90474987
H	14.38390950	-3.04802344	0.51138331

**f. Transition State 5**

C	2.19855815	1.24459861	-0.25206097
C	4.31383553	0.03242621	-0.06238269
C	6.44786674	-1.20214472	-0.07817025
C	8.57634878	-2.44351269	-0.17377744
C	10.68497660	-3.67242143	-0.47540214
C	4.33208915	2.46999081	0.15397012
C	6.44514495	1.26326987	-0.06771985
C	9.99447291	0.03096568	-0.15120073
C	10.70506131	-1.20392577	-0.26199053
C	12.80487511	-2.45800123	-0.46549570
C	6.45866285	3.70408466	-0.25084601
C	8.57591239	2.49355204	-0.06753999
C	10.70633488	1.25821049	-0.13193466
C	12.83425864	0.02607666	-0.35168919
C	14.93489233	-1.23349061	-0.10105494
C	8.59373670	4.92970230	0.14890259
C	10.70682884	3.72399708	-0.07950057

C	12.83784574	2.48528326	-0.14386402
C	14.96588356	1.24749327	-0.14992860
C	17.13394521	0.01466055	-0.21368165
C	3.59492913	1.28241002	-0.05130500
C	5.73485352	0.03444650	-0.04748413
C	7.86417341	-1.20412222	-0.11256178
C	9.98868448	-2.43634946	-0.28313305
C	12.08930134	-3.66160553	-0.41203707
C	5.72599804	2.51213538	-0.05749642
C	7.86341597	1.26400541	-0.09545609
C	12.10837962	-1.20676882	-0.39446964
C	14.22871026	-2.46314770	-0.48956771
C	7.85603789	3.74281101	-0.05526905
C	9.99479098	2.49510695	-0.06527808
C	12.12465312	1.25835039	-0.22310111
C	14.24022951	0.04579644	-0.29603049
C	16.40202879	-1.21467905	0.17612241
C	9.98768110	4.97178402	-0.06253827
C	12.12536851	3.72489316	-0.10496525
C	14.25840617	2.48743166	-0.12174109
C	16.40423126	1.24446852	-0.10895621
C	18.43957408	0.06663683	-0.66426351
Br	17.42685871	-2.89492707	0.44672662
Br	14.99486340	-3.46986253	-1.93103432
Br	13.01214158	-5.23561756	0.16949261
Br	7.77372649	6.36068271	1.11245787
Br	5.62669849	5.14566266	-1.18760669
Br	3.51086233	3.89216001	1.13066550
Br	1.36801834	2.68751077	-1.18768322
Br	19.08902780	-1.25314078	-1.88530035
C	8.57504434	0.02598139	-0.10906719
O	15.56977983	-1.07487896	1.28519269
O	15.30104522	-1.79040481	3.92841137

H	16.01793537	-2.07378284	3.33917556
H	14.54121616	-1.77471530	3.29453136
O	13.47020476	-2.32201145	2.09689784
H	12.84361068	-2.70235743	2.75953104
H	13.96333567	-2.84692249	1.26952143

**g. Final**

C	2.16918294	1.19394193	-0.20297449
C	4.28942800	-0.01831412	-0.06984040
C	6.42652014	-1.24829287	-0.08988272
C	8.56504679	-2.49053142	-0.12250120
C	10.69360539	-3.73221671	-0.30793714
C	4.30493118	2.41396284	0.20077803
C	6.41900406	1.21542605	-0.06661855
C	9.97665081	-0.02324926	-0.10129094
C	10.69805196	-1.26216096	-0.13307466
C	12.82398665	-2.51505777	-0.31005392
C	6.42911094	3.65506249	-0.19902375
C	8.55012156	2.44398432	-0.06340954
C	10.68038003	1.21006922	-0.10982279
C	12.81465133	-0.01579868	-0.28084216
C	14.91799369	-1.27546097	-0.10916241
C	8.56726590	4.87498200	0.19878242
C	10.68077422	3.67510327	-0.07784198
C	12.81524904	2.44041108	-0.16392775
C	14.95013877	1.20392132	-0.15479368
C	17.12386493	-0.03233688	-0.11008512
C	3.56898114	1.22840201	-0.02250580
C	5.71062698	-0.01341816	-0.06065637
C	7.84564968	-1.25178152	-0.10092919
C	9.98245745	-2.49460402	-0.16942337
C	12.09863919	-3.71833913	-0.19882903
C	5.69700350	2.46259730	-0.02407932
C	7.83777542	1.21631303	-0.09796282

C	12.10611262	-1.25975169	-0.23534744
C	14.21375671	-2.46601098	-0.53360774
C	7.82935504	3.69054945	-0.02089890
C	9.96799260	2.44731626	-0.06642573
C	12.09873322	1.21587165	-0.19719009
C	14.22274212	0.00654096	-0.28836082
C	16.36110586	-1.25659187	0.25883169
C	9.95959224	4.92188072	-0.02870550
C	12.09917244	3.67748826	-0.12022928
C	14.23734240	2.44089434	-0.14012627
C	16.38808723	1.19924160	-0.07913230
C	18.45729745	-0.00111171	-0.49638333
Br	17.38056106	-2.93096656	0.59870084
Br	15.01662482	-3.59594961	-1.82386102
Br	13.01878881	-5.24462891	0.47216375
Br	7.75869138	6.28005259	1.20946563
Br	5.58588706	5.11670777	-1.09709448
Br	3.49282400	3.81621340	1.21254222
Br	1.32790025	2.65545587	-1.10285389
Br	19.16329395	-1.34661968	-1.65960452
C	8.55378514	-0.02138628	-0.09919816
O	15.46461506	-1.13736588	1.32368615
O	15.86628062	-1.44063338	4.09788347
H	16.23979965	-1.85613704	3.30341306
H	14.90568325	-1.55307876	3.96038636
O	13.12737279	-1.96934281	3.22089480
H	12.26426479	-1.77468642	3.61462736
H	13.09296104	-1.59154284	2.32923393

**3) OH formation**  
**a. Initial**

C	2.16798452	1.18868762	-0.20278841
C	4.28718748	-0.02363138	-0.06331446
C	6.42137192	-1.25408763	-0.08276492

C	8.55307294	-2.49171549	-0.15456229
C	10.67824499	-3.71760214	-0.43296162
C	4.30180565	2.41002517	0.19754661
C	6.41508783	1.21070015	-0.06503947
C	9.96985388	-0.02334192	-0.12740673
C	10.68638306	-1.25949186	-0.20330644
C	12.78496967	-2.51633659	-0.32148901
C	6.42749016	3.65075768	-0.19694483
C	8.54797336	2.43950721	-0.06322571
C	10.67813185	1.20555020	-0.11245821
C	12.81744331	-0.02775151	-0.26033707
C	14.93072373	-1.27645958	-0.03894465
C	8.56565504	4.87060095	0.19412285
C	10.68006831	3.66942772	-0.07361800
C	12.81500125	2.43199353	-0.13310827
C	14.94930218	1.19140438	-0.10972496
C	17.12894369	-0.03541302	-0.21838823
C	3.56770862	1.22222346	-0.02165180
C	5.70710795	-0.01861375	-0.05638370
C	7.83866716	-1.25468169	-0.10985851
C	9.97311570	-2.48769590	-0.24673798
C	12.09059778	-3.71110794	-0.33425663
C	5.69495593	2.45708066	-0.02347763
C	7.83429909	1.21303731	-0.09788787
C	12.09529456	-1.27204526	-0.28127012
C	14.25052036	-2.52463950	-0.46191924
C	7.82869567	3.68493101	-0.02053387
C	9.96661892	2.44158051	-0.06558034
C	12.10024109	1.20592441	-0.17535154
C	14.22204274	-0.00519991	-0.22755348
C	16.40248571	-1.28401700	0.12148102
C	9.95956674	4.91546506	-0.02956934
C	12.09838036	3.67122766	-0.10757080



C	14.23780190	2.43066023	-0.10869506
C	16.39076066	1.19185664	-0.09158263
C	18.43926985	0.02809698	-0.67045956
Br	17.36696031	-3.00601649	0.12990494
Br	14.63504303	-2.63261049	-2.47207819
Br	13.05476602	-5.33007631	0.00299121
Br	7.75589137	6.28075246	1.20102946
Br	5.58595070	5.11089502	-1.10388597
Br	3.48639291	3.81771232	1.20295166
Br	1.32741369	2.64789721	-1.11164947
Br	19.07096942	-1.20215054	-1.99661701
C	8.54887752	-0.02325422	-0.10998114
O	15.60373711	-1.23084696	1.29728290
H	14.30498382	-2.09608549	2.55815850
O	13.43165726	-2.51651174	2.62700010
H	12.94363119	-1.96530282	3.25751508
H	14.73189012	-3.41753825	-0.06401208

**b. Transition State 1**

C	2.16782750	1.19205927	-0.20273345
C	4.28719297	-0.01565309	-0.05730842
C	6.42064675	-1.24143525	-0.09709597
C	8.54912789	-2.46764740	-0.21310730
C	10.67149059	-3.71987775	-0.40984519
C	4.29885393	2.41741679	0.20703317
C	6.41271961	1.22122402	-0.06291216
C	9.96743240	-0.01563198	-0.16345570
C	10.68192468	-1.25254716	-0.23567170
C	12.78462698	-2.51410294	-0.18778415
C	6.42507608	3.65891244	-0.19055759
C	8.54634161	2.44877394	-0.06416285
C	10.67675216	1.21124206	-0.11918912
C	12.81350019	-0.02717974	-0.19598624
C	14.93204982	-1.23814985	0.07032139

C	8.56471763	4.87820561	0.20344470
C	10.67822284	3.67457395	-0.06793089
C	12.81302895	2.43893498	-0.11600122
C	14.95685552	1.21418488	-0.06745461
C	17.11378338	-0.00873904	-0.11367923
C	3.56802728	1.22759006	-0.01435764
C	5.70632449	-0.00895979	-0.05681532
C	7.83498412	-1.23714335	-0.15852431
C	9.97112960	-2.47820855	-0.28576269
C	12.07754813	-3.71272122	-0.20703999
C	5.69212563	2.46532303	-0.01349027
C	7.83230038	1.22377137	-0.10698748
C	12.09750897	-1.26689022	-0.24593552
C	14.25840104	-2.52091641	-0.11124985
C	7.82714664	3.69298613	-0.01410236
C	9.96564866	2.44692887	-0.06738317
C	12.10037825	1.20757006	-0.15092248
C	14.23421801	-0.02064106	-0.09484863
C	16.33649517	-1.12749349	0.58047124
C	9.95841043	4.91954441	-0.02185533
C	12.09876835	3.67497618	-0.10190612
C	14.24156133	2.43875339	-0.10080574
C	16.38860022	1.22674069	-0.08424237
C	18.40902141	0.01254423	-0.59099203
Br	17.33819768	-2.98371757	0.66572361
Br	14.93623734	-2.95908242	-2.03551875
Br	13.01187247	-5.30795192	0.24789760
Br	7.75955098	6.29165873	1.20566692
Br	5.58368558	5.11751214	-1.09544674
Br	3.47750654	3.82238105	1.20824804
Br	1.33179641	2.64371135	-1.12153062
Br	19.05045519	-1.37995529	-1.72002342
C	8.54651029	-0.00914850	-0.14629961

O	16.07149568	-0.76935036	1.82835750
H	14.83102819	-1.81147723	2.55219771
O	14.02110770	-2.37029029	2.64467022
H	13.34259625	-1.73727775	2.92257746
H	14.68570137	-3.32449589	0.48580241

**c. Transition State 2**

C	2.16147832	1.19209238	-0.20325904
C	4.27931288	-0.01538837	-0.05480615
C	6.41042373	-1.24057883	-0.09320021
C	8.53616266	-2.46546700	-0.20862978
C	10.65020449	-3.71627045	-0.41725860
C	4.29142897	2.41796377	0.20915045
C	6.40418057	1.22234682	-0.05881478
C	9.95655886	-0.01389255	-0.16247842
C	10.66701412	-1.24913912	-0.24874195
C	12.76634753	-2.50999172	-0.23895147
C	6.41868403	3.65979730	-0.19147343
C	8.53854750	2.44961619	-0.06062403
C	10.66771255	1.21143116	-0.12134096
C	12.80442750	-0.02746261	-0.24324858
C	14.92560326	-1.23905904	-0.01424338
C	8.55727735	4.87885305	0.20629872
C	10.67015981	3.67489583	-0.06557451
C	12.80403103	2.43900665	-0.12554129
C	14.94657174	1.21557152	-0.09329894
C	17.10034173	-0.00836855	-0.10297626
C	3.56135095	1.22774902	-0.01279118
C	5.69751254	-0.00818647	-0.05255897
C	7.82417570	-1.23536416	-0.15137871
C	9.95592612	-2.47433559	-0.29286850
C	12.05363355	-3.70716621	-0.20889895
C	5.68473439	2.46638258	-0.01258922
C	7.82380289	1.22524255	-0.10231903

C	12.08208854	-1.26448655	-0.28402342
C	14.24116163	-2.52902046	-0.09618165
C	7.82036317	3.69361819	-0.01258320
C	9.95764067	2.44700030	-0.06442735
C	12.09131761	1.20679472	-0.17037766
C	14.22920850	-0.02331610	-0.16477412
C	16.31274063	-1.13013424	0.56676683
C	9.95103467	4.91990074	-0.01937761
C	12.09096849	3.67486057	-0.10195908
C	14.23171407	2.44009697	-0.11065331
C	16.37615543	1.22851195	-0.08432203
C	18.39314498	0.01093599	-0.58115555
Br	17.35841759	-2.93545153	0.75603550
Br	15.03435426	-3.38248153	-1.77951851
Br	12.93860276	-5.27818643	0.39834735
Br	7.75093230	6.29386337	1.20451044
Br	5.57824098	5.11728666	-1.09820328
Br	3.47005311	3.82319281	1.20860053
Br	1.32624092	2.64226575	-1.12399065
Br	19.05796061	-1.39741333	-1.67590975
C	8.53673569	-0.00722921	-0.13813845
O	15.98618791	-0.77875672	1.80785443
H	14.85988554	-1.81011488	2.52624739
O	14.12093825	-2.46374457	2.65699525
H	13.33882503	-1.91258437	2.81394725
H	14.52696125	-3.13634398	0.77330454

**d. Transition State 3**

C	2.16002760	1.19370909	-0.20497577
C	4.27750771	-0.01358521	-0.05462631
C	6.40758681	-1.23965762	-0.08894924
C	8.53231260	-2.46443857	-0.20268475
C	10.64315249	-3.71497207	-0.42341120
C	4.29023444	2.41937740	0.20887135

C	6.40224395	1.22375691	-0.05983251
C	9.95254629	-0.01223378	-0.15530454
C	10.66052861	-1.24710585	-0.24757142
C	12.76029242	-2.50581583	-0.28384325
C	6.41734862	3.66134607	-0.19398439
C	8.53623685	2.45098402	-0.06033120
C	10.66484428	1.21314725	-0.11553693
C	12.79996868	-0.02529275	-0.24454764
C	14.92315835	-1.24271657	-0.07649314
C	8.55622059	4.88004192	0.20621110
C	10.66810927	3.67647711	-0.06519536
C	12.80125713	2.44067842	-0.11910493
C	14.94353960	1.21707330	-0.08343732
C	17.09446130	-0.00823294	-0.09718475
C	3.55990312	1.22920436	-0.01362054
C	5.69520627	-0.00690561	-0.05189112
C	7.82123988	-1.23443356	-0.14529508
C	9.95074175	-2.47225336	-0.29496228
C	12.04583660	-3.70404680	-0.22947140
C	5.68341262	2.46762848	-0.01435590
C	7.82161712	1.22667632	-0.10153030
C	12.07514394	-1.26061218	-0.29411119
C	14.22892328	-2.51615501	-0.13369592
C	7.81882573	3.69471270	-0.01360877
C	9.95526876	2.44856715	-0.06236118
C	12.08799168	1.20888070	-0.16328359
C	14.22568294	-0.02185955	-0.17012547
C	16.30272027	-1.13206223	0.55637852
C	9.94954264	4.92122651	-0.02069890
C	12.08904063	3.67641117	-0.09972892
C	14.22897884	2.44128338	-0.10173017
C	16.37123517	1.22967818	-0.07793284
C	18.38576095	0.00992097	-0.57651248

Br	17.36958748	-2.91531654	0.77929544
Br	15.08245608	-3.56804140	-1.62810952
Br	12.91648325	-5.26526242	0.42777926
Br	7.75033281	6.29358082	1.20603253
Br	5.57685230	5.11827008	-1.10007347
Br	3.46987056	3.82293941	1.21037954
Br	1.32433927	2.64380966	-1.12435610
Br	19.05365757	-1.40111651	-1.66733368
C	8.53382019	-0.00585684	-0.13241079
O	15.97699044	-0.77512440	1.80176428
H	14.94930216	-1.76143744	2.38306502
O	14.26336516	-2.51445094	2.52170913
H	13.39925732	-2.08115890	2.55270169
H	14.39410101	-2.93843970	0.94038940

**e. Transition State 4**

C	2.15952111	1.19438715	-0.20178474
C	4.27690500	-0.01384529	-0.05509037
C	6.40663053	-1.24216707	-0.09036130
C	8.53226215	-2.46835486	-0.20046323
C	10.64364002	-3.72136467	-0.42262874
C	4.29049147	2.41866768	0.20681703
C	6.40279240	1.22253602	-0.05984955
C	9.95255601	-0.01328296	-0.15328040
C	10.66131597	-1.24960077	-0.24000671
C	12.77173512	-2.50551506	-0.30487217
C	6.41746239	3.66046035	-0.19174620
C	8.53643104	2.45039200	-0.06044657
C	10.66514080	1.21392314	-0.11631749
C	12.79799745	-0.02295896	-0.23240128
C	14.90691285	-1.26529979	-0.10192239
C	8.55641002	4.87971561	0.20411899
C	10.66842632	3.67693912	-0.06531384
C	12.80024568	2.44125092	-0.11916324

C	14.93936372	1.21056650	-0.06186439
C	17.08457664	-0.01715413	-0.07167752
C	3.55901648	1.23003226	-0.01417843
C	5.69467936	-0.00776138	-0.05326788
C	7.82130566	-1.23611372	-0.14512123
C	9.94992796	-2.47410932	-0.29416336
C	12.04434139	-3.71063468	-0.24730427
C	5.68348947	2.46761935	-0.01421862
C	7.82152333	1.22609041	-0.10187613
C	12.07708366	-1.25682574	-0.27767188
C	14.22021847	-2.46472733	-0.31927964
C	7.81843372	3.69489034	-0.01380866
C	9.95513110	2.44978796	-0.06315000
C	12.08561513	1.21370570	-0.16368853
C	14.21422716	-0.02305657	-0.12822185
C	16.27974941	-1.15519835	0.55554776
C	9.94916921	4.92284324	-0.02129104
C	12.08783059	3.67808750	-0.09952302
C	14.22624255	2.43947989	-0.09940842
C	16.36718982	1.22508272	-0.06672487
C	18.37858611	-0.00032927	-0.55950511
Br	17.35639349	-2.91213858	0.77409271
Br	15.09219867	-3.61599336	-1.61318325
Br	12.92261161	-5.26670969	0.42502791
Br	7.74919124	6.29511146	1.20468523
Br	5.57611690	5.11949940	-1.09888661
Br	3.46908412	3.82500824	1.20864695
Br	1.32308671	2.64665806	-1.12324220
Br	19.05143145	-1.40343682	-1.66228947
C	8.53421141	-0.00789579	-0.13322823
O	15.93529848	-0.82903952	1.84526190
H	15.13145326	-1.62556642	2.25142738
O	14.26655825	-2.57955843	2.36890030

H	13.41775218	-2.12331430	2.54190415
H	14.29405002	-2.83686058	1.31689217

**f. Transition State 5**

C	2.17225065	1.19850744	-0.20712568
C	4.29264147	-0.01112484	-0.05842090
C	6.42820131	-1.24381996	-0.07706680
C	8.56205485	-2.47111352	-0.18203935
C	10.69661752	-3.71282041	-0.44707984
C	4.30793971	2.42068084	0.19285279
C	6.42118595	1.22067924	-0.06696731
C	9.97647871	-0.01329196	-0.12880504
C	10.69329500	-1.24916776	-0.22552587
C	12.83431371	-2.46931678	-0.46828116
C	6.43188386	3.66011223	-0.20358259
C	8.55203276	2.45105690	-0.06250968
C	10.68409902	1.21836850	-0.09938067
C	12.82018776	-0.00927552	-0.18712883
C	14.94424027	-1.26542712	-0.13933273
C	8.57036292	4.88210914	0.19181062
C	10.68384774	3.68097272	-0.06751013
C	12.81807526	2.44709653	-0.09202212
C	14.96005827	1.20801506	-0.00415547
C	17.12770745	-0.00864331	-0.11269707
C	3.57283218	1.23310963	-0.02360468
C	5.71277805	-0.00853424	-0.05476478
C	7.84592692	-1.23891998	-0.12354590
C	9.98271633	-2.47576382	-0.28842306
C	12.11189621	-3.68571428	-0.39308747
C	5.70076814	2.46606948	-0.02759114
C	7.83995353	1.22459407	-0.09940364
C	12.11176055	-1.24007637	-0.29349954
C	14.26950902	-2.38066538	-0.61019660
C	7.83244361	3.69602990	-0.02291078



C	9.97138412	2.45371517	-0.06066821
C	12.10479213	1.22269182	-0.12354075
C	14.23037134	-0.02130645	-0.07003345
C	16.33605622	-1.15847030	0.48229529
C	9.96367012	4.92617010	-0.02971636
C	12.10300604	3.68280255	-0.09460449
C	14.24470757	2.43862495	-0.06089129
C	16.39380293	1.22324999	-0.06011908
C	18.43958773	0.00392937	-0.55703583
Br	17.30602254	-2.92153212	0.71520477
Br	15.16176010	-3.62915034	-1.75029352
Br	13.03159395	-5.23690933	0.25519150
Br	7.75865398	6.29688460	1.19051806
Br	5.59110040	5.11825136	-1.11382533
Br	3.49044716	3.83098297	1.19310184
Br	1.33552561	2.65386827	-1.12551705
Br	19.08628272	-1.42229166	-1.65437557
C	8.55561438	-0.01000845	-0.11637341
O	16.13417345	-0.73435682	1.82079612
H	15.51414335	-1.37774408	2.24804354
O	13.93172880	-2.40610890	2.69218104
H	13.16913244	-1.84797915	2.91286878
H	13.76492392	-2.65923409	1.76809790

**g. Final**

C	2.18077226	1.20108508	-0.21792452
C	4.30051021	-0.00912268	-0.06250123
C	6.43542927	-1.24242577	-0.07708982
C	8.56906232	-2.47177954	-0.17788279
C	10.70522051	-3.71304918	-0.42854955
C	4.31746363	2.42397049	0.17947097
C	6.43002750	1.22203906	-0.07116003
C	9.98419128	-0.01247261	-0.12783976
C	10.70071597	-1.24854548	-0.22297833

C	12.84126409	-2.47136087	-0.45220196
C	6.44120692	3.66240824	-0.21609731
C	8.56015378	2.45310539	-0.06491751
C	10.69140262	1.21988483	-0.09889377
C	12.82514399	-0.00968937	-0.18729338
C	14.94257475	-1.26660998	-0.14492693
C	8.57928892	4.88536561	0.18045546
C	10.69235099	3.68281061	-0.07021261
C	12.82490056	2.44823887	-0.09263686
C	14.96465859	1.20867017	-0.00687965
C	17.13103952	-0.01306932	-0.09799762
C	3.58103069	1.23607769	-0.03308611
C	5.72069753	-0.00646620	-0.05680675
C	7.85321605	-1.23848340	-0.12299899
C	9.99014444	-2.47529627	-0.28271418
C	12.12032579	-3.68620107	-0.36712478
C	5.71054483	2.46797285	-0.03780120
C	7.84840784	1.22600033	-0.10068602
C	12.11945549	-1.24174755	-0.28882690
C	14.27078370	-2.38961842	-0.58920449
C	7.84083609	3.69898460	-0.03105936
C	9.97942645	2.45572834	-0.06103648
C	12.11194649	1.22306760	-0.12325891
C	14.23524832	-0.02081099	-0.07437802
C	16.32371797	-1.17207838	0.46813010
C	9.97298863	4.92838886	-0.03761344
C	12.11086936	3.68429466	-0.09608006
C	14.25088519	2.44036546	-0.06223924
C	16.39801184	1.22322185	-0.05630609
C	18.44941653	0.00085877	-0.52939545
Br	17.31535663	-2.89822813	0.74272146
Br	15.17408350	-3.66616910	-1.69015714
Br	13.02532817	-5.22385234	0.31994232

Br	7.76375644	6.30377500	1.17222778
Br	5.60396521	5.11538941	-1.13833398
Br	3.49895562	3.83969996	1.17227083
Br	1.34466980	2.65268622	-1.14354825
Br	19.09962247	-1.42138521	-1.63535427
C	8.56318105	-0.00929432	-0.11609283
O	15.98769400	-0.80639515	1.83066866
H	16.81704180	-0.79931078	2.34643493
O	13.49714995	-2.50427685	2.81724466
H	12.91693464	-1.77770480	3.08765114
H	14.32279609	-2.05859634	2.55482874

#### 4) HOH formation

##### a. Initial

C	2.18049329	1.19659477	-0.21644849
C	4.29935083	-0.01071328	-0.06414014
C	6.43388471	-1.23837964	-0.08981926
C	8.56667370	-2.47061406	-0.19045631
C	10.69651762	-3.73153206	-0.35576615
C	4.31543944	2.41941011	0.19610246
C	6.42726196	1.22362020	-0.07221087
C	9.98078228	-0.01517777	-0.16797650
C	10.69545941	-1.25141307	-0.23951756
C	12.81991618	-2.48920277	-0.26725637
C	6.43931609	3.66087988	-0.20882826
C	8.55915960	2.45060129	-0.07143871
C	10.69066498	1.21495423	-0.12789720
C	12.82161836	-0.01605658	-0.22521826
C	14.92858431	-1.22924186	0.03407490
C	8.57984527	4.87955186	0.19275889
C	10.69046794	3.67883989	-0.07630690
C	12.82367000	2.44738905	-0.11411578
C	14.96454207	1.22277559	-0.03125351
C	17.11203277	-0.01386258	-0.04575947

C	3.57971758	1.23314630	-0.02654356
C	5.71943889	-0.00571748	-0.06028233
C	7.85147268	-1.23863846	-0.14789812
C	9.98841887	-2.48357516	-0.26302872
C	12.11380308	-3.69330635	-0.23648066
C	5.70743212	2.46823851	-0.02861321
C	7.84625746	1.22389919	-0.11195344
C	12.11360821	-1.25095049	-0.27662172
C	14.28798402	-2.48143870	-0.25946304
C	7.83968394	3.69638806	-0.02677151
C	9.97914602	2.45019764	-0.07171220
C	12.11430323	1.21351823	-0.16271090
C	14.24932794	-0.02027496	-0.09225039
C	16.30963677	-1.13936255	0.60648460
C	9.97234003	4.92363134	-0.03466540
C	12.11167303	3.67874502	-0.10650899
C	14.25152664	2.44494512	-0.08209712
C	16.39124686	1.22668813	-0.05655248
C	18.43480832	-0.00987083	-0.47432736
Br	17.23544646	-2.92236134	0.74385797
Br	14.89577592	-2.93642140	-2.31981078
Br	13.09296554	-5.27810079	0.19279835
Br	7.77398622	6.29159509	1.19638254
Br	5.59869939	5.11915278	-1.11303129
Br	3.49676641	3.82464800	1.19843382
Br	1.34504047	2.64686840	-1.13685866
Br	19.05880147	-1.43248468	-1.58383486
C	8.55957221	-0.00950622	-0.14438913
O	16.10849582	-0.73773061	1.98327317
H	16.99014333	-0.69400137	2.39768862
H	14.52891054	-1.77779212	2.56854637
O	13.73766076	-2.34692522	2.63168922
H	13.15739842	-1.88307389	3.25407020

H	14.73057309	-3.34248983	0.23683950
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**b. Transition State 1**

C	2.17144615	1.18742992	-0.22507856
C	4.28739650	-0.02212812	-0.06486681
C	6.41641442	-1.25169476	-0.09389467
C	8.54416766	-2.47425459	-0.21615242
C	10.66561395	-3.72731968	-0.36546669
C	4.30435046	2.41078283	0.18675626
C	6.41489150	1.21337009	-0.07115098
C	9.96727015	-0.02377375	-0.16229838
C	10.67768049	-1.25902215	-0.24072953
C	12.78845276	-2.51956202	-0.20573341
C	6.43121398	3.65175698	-0.21809425
C	8.54911949	2.44134082	-0.06845443
C	10.67957689	1.20288136	-0.12120023
C	12.81141777	-0.04063317	-0.24959718
C	14.93230575	-1.25460191	-0.01840437
C	8.56986796	4.87099116	0.18563906
C	10.68045826	3.66806683	-0.07665961
C	12.81200172	2.43082961	-0.12632272
C	14.95283313	1.20229096	-0.09248746
C	17.09609339	-0.01954329	-0.10577005
C	3.57000996	1.22274325	-0.03156359
C	5.70566426	-0.01732813	-0.05816623
C	7.83226252	-1.24466304	-0.15457143
C	9.96405756	-2.48335695	-0.27780263
C	12.06615065	-3.70820018	-0.14259932
C	5.69674173	2.45941654	-0.03534420
C	7.83436649	1.21573677	-0.10781120
C	12.09688321	-1.27318080	-0.27758026
C	14.26081103	-2.53872530	-0.10385115
C	7.83091350	3.68682636	-0.03080771
C	9.96923984	2.43928230	-0.06746144

C	12.10388566	1.19335583	-0.17151171
C	14.24728753	-0.05194260	-0.16582293
C	16.30651114	-1.12838650	0.55747308
C	9.96277131	4.91392478	-0.04046094
C	12.10188045	3.66498169	-0.10910464
C	14.23919235	2.42636277	-0.10590749
C	16.37496751	1.21916934	-0.10430397
C	18.42224058	-0.00542773	-0.52922736
Br	17.28666172	-2.83283365	0.77975286
Br	14.97755277	-3.52253529	-1.86352130
Br	12.92007277	-5.26936738	0.55061353
Br	7.75946674	6.28899006	1.17479929
Br	5.59764275	5.10112066	-1.14281814
Br	3.48267311	3.82522120	1.17185909
Br	1.33921694	2.63034639	-1.15946659
Br	19.12705824	-1.39174254	-1.63740428
C	8.54594431	-0.01681118	-0.13897260
O	16.05617024	-0.63237113	1.97624829
H	16.79298619	-0.91662905	2.55295529
H	14.64548133	-1.54237472	2.55546616
O	13.98493995	-2.26247218	2.66512392
H	13.15238393	-1.83265948	2.88740688
H	14.59504219	-3.22874089	0.66740941

**c. Transition State 2**

C	2.16967016	1.18668687	-0.22492545
C	4.28519295	-0.02399107	-0.06456096
C	6.41251784	-1.25515343	-0.09273221
C	8.53725364	-2.48177650	-0.22176680
C	10.66079180	-3.72765459	-0.35965668
C	4.30217900	2.41041255	0.18486921
C	6.41279282	1.21108683	-0.07015712
C	9.96300677	-0.02565805	-0.15478960
C	10.67108722	-1.26130045	-0.23285634

C	12.77688365	-2.52251013	-0.20122640
C	6.42964719	3.65060077	-0.21850510
C	8.54721139	2.43896648	-0.06764365
C	10.67622146	1.20055176	-0.11458915
C	12.80841034	-0.04314984	-0.24796533
C	14.94161567	-1.25903692	-0.09283350
C	8.56779860	4.87026173	0.18347667
C	10.67851112	3.66626793	-0.07572289
C	12.80921224	2.42846347	-0.12262654
C	14.94570116	1.19681608	-0.13039004
C	17.08036665	-0.03243435	-0.20160227
C	3.56810361	1.22197065	-0.03193035
C	5.70300925	-0.01962142	-0.05658711
C	7.82858064	-1.24988419	-0.14906405
C	9.95695791	-2.48562463	-0.27149519
C	12.05831605	-3.70904494	-0.12366965
C	5.69505411	2.45774495	-0.03621310
C	7.83194092	1.21331764	-0.10486704
C	12.08905308	-1.27604000	-0.27479333
C	14.24874689	-2.55227923	-0.09287893
C	7.82931679	3.68488801	-0.03115606
C	9.96683148	2.43732377	-0.06558560
C	12.09992678	1.19139391	-0.16234935
C	14.24169761	-0.04687883	-0.21174420
C	16.32350657	-1.18400001	0.25595113
C	9.96089587	4.91283262	-0.04157779
C	12.09884087	3.66440565	-0.10658737
C	14.23333371	2.42594200	-0.11189396
C	16.36386029	1.20916691	-0.15267867
C	18.42822267	0.00580897	-0.57691079
Br	17.27637651	-2.78210022	0.71788568
Br	14.94874370	-3.61862527	-1.75008246
Br	12.89633903	-5.26021395	0.60479277

Br	7.75856985	6.28750028	1.17238647
Br	5.59813512	5.09925284	-1.14470526
Br	3.48273759	3.82492151	1.16930813
Br	1.33756996	2.63037458	-1.15808888
Br	19.17041367	-1.35828956	-1.68394825
C	8.54254640	-0.02066836	-0.13139876
O	15.93460114	-0.47564467	2.21314363
H	16.66371681	-0.87966640	2.72159143
H	14.74439979	-1.51059288	2.55957778
O	14.12006821	-2.30703558	2.66081609
H	13.23700092	-1.94870468	2.81016170
H	14.54018776	-3.12034408	0.79861393

**d. Transition State 3**

C	2.16975959	1.18739253	-0.22468226
C	4.28518810	-0.02506035	-0.06497848
C	6.41108241	-1.25829716	-0.09181602
C	8.53474546	-2.48961600	-0.22708414
C	10.66108132	-3.72886426	-0.35162740
C	4.30235289	2.41099190	0.18048830
C	6.41297697	1.20903581	-0.07048044
C	9.96152724	-0.02690911	-0.14965495
C	10.66813483	-1.26287439	-0.22788983
C	12.77228996	-2.52148661	-0.21521511
C	6.43007738	3.65010030	-0.21820420
C	8.54742525	2.43685119	-0.06818073
C	10.67629563	1.19914643	-0.11046816
C	12.81036636	-0.04402564	-0.24183476
C	14.95582046	-1.26785392	-0.16020137
C	8.56784041	4.87053782	0.17901858
C	10.67887155	3.66550450	-0.07545666
C	12.80917143	2.42725171	-0.11767812
C	14.94112150	1.19197387	-0.15517926
C	17.07371518	-0.04022519	-0.27840553



C	3.56776886	1.22253544	-0.03376501
C	5.70253217	-0.02112943	-0.05624627
C	7.82809230	-1.25495168	-0.14583501
C	9.95340613	-2.48809702	-0.26675633
C	12.05883343	-3.70725415	-0.11619411
C	5.69558090	2.45689867	-0.03788111
C	7.83167468	1.21146681	-0.10337225
C	12.08473297	-1.27631666	-0.27474929
C	14.24136569	-2.55422201	-0.07678996
C	7.82970885	3.68418694	-0.03270170
C	9.96672678	2.43630628	-0.06505998
C	12.09997575	1.19105642	-0.15300518
C	14.23946931	-0.04294349	-0.23270187
C	16.34326791	-1.23750932	-0.01170917
C	9.96119869	4.91323396	-0.04346556
C	12.09786787	3.66540714	-0.10400062
C	14.22967661	2.42606281	-0.11302908
C	16.35701957	1.19833977	-0.20518580
C	18.44113024	0.01297261	-0.59983325
Br	17.27795809	-2.76325764	0.64944905
Br	14.93951206	-3.71221938	-1.62919337
Br	12.88184930	-5.24981052	0.64261673
Br	7.75874572	6.28747108	1.16877206
Br	5.59833473	5.09869390	-1.14463744
Br	3.48382294	3.82564879	1.16602147
Br	1.33739227	2.63186954	-1.15711843
Br	19.20546624	-1.33560265	-1.70996104
C	8.54191531	-0.02457562	-0.12675065
O	15.79872826	-0.48906028	2.44666537
H	16.62851492	-0.88868273	2.75893645
H	14.87851918	-1.47083436	2.57604058
O	14.19116281	-2.33766650	2.64261665
H	13.28311701	-2.01160278	2.71613532

H	14.43856655	-2.95091766	0.96973415
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**e. Transition State 4**

C	2.16946501	1.18778643	-0.22372048
C	4.28518250	-0.02512274	-0.06488151
C	6.41139286	-1.25930372	-0.09196203
C	8.53562143	-2.49141778	-0.22727177
C	10.66530512	-3.73139120	-0.35208023
C	4.30242121	2.41114500	0.17963911
C	6.41328406	1.20859389	-0.07073352
C	9.96155182	-0.02719320	-0.14867588
C	10.66856051	-1.26400900	-0.22385828
C	12.78204611	-2.52195313	-0.23021325
C	6.42994769	3.65021991	-0.21716754
C	8.54738796	2.43646964	-0.06804000
C	10.67718247	1.19920971	-0.11103994
C	12.81228412	-0.04495536	-0.23815631
C	14.95426472	-1.27931057	-0.17475775
C	8.56809091	4.87030667	0.17803475
C	10.67874196	3.66540415	-0.07542579
C	12.80921343	2.42698246	-0.11760358
C	14.94025261	1.18951074	-0.15032151
C	17.07179493	-0.04588916	-0.28010973
C	3.56756506	1.22292372	-0.03370022
C	5.70248473	-0.02124516	-0.05729696
C	7.82836722	-1.25556885	-0.14505515
C	9.95412965	-2.48832745	-0.26721613
C	12.06002881	-3.71234967	-0.12825926
C	5.69557391	2.45712373	-0.03791947
C	7.83162049	1.21146718	-0.10344471
C	12.08601366	-1.27508083	-0.26688850
C	14.23467718	-2.53878638	-0.14415165
C	7.82952009	3.68424894	-0.03296237
C	9.96663787	2.43675334	-0.06523733

C	12.09926708	1.19332135	-0.15443070
C	14.23814307	-0.04319907	-0.22000219
C	16.34781330	-1.24157901	-0.03070366
C	9.96091917	4.91378452	-0.04366205
C	12.09752545	3.66594683	-0.10363021
C	14.22955237	2.42583666	-0.11067565
C	16.35554666	1.19625698	-0.20385906
C	18.44310053	0.01079765	-0.59736001
Br	17.27719698	-2.76424079	0.64938171
Br	14.94965381	-3.72752960	-1.60350754
Br	12.88560237	-5.25165909	0.63833026
Br	7.75811915	6.28821398	1.16835007
Br	5.59781511	5.09918451	-1.14354674
Br	3.48348607	3.82622751	1.16547003
Br	1.33656293	2.63308363	-1.15651572
Br	19.20410621	-1.33716947	-1.71166617
C	8.54240887	-0.02534957	-0.12698418
O	15.75502380	-0.52570976	2.47417800
H	16.60690179	-0.89623174	2.75554830
H	15.04562538	-1.33792480	2.55604121
O	14.18888475	-2.45813469	2.49017735
H	13.30170170	-2.08207195	2.65922026
H	14.34145454	-2.81861954	1.23723019

**f. Transition State 5**

C	2.17372572	1.18728691	-0.22139979
C	4.29081936	-0.02591049	-0.06606037
C	6.42016727	-1.26257198	-0.09077156
C	8.54927133	-2.49946466	-0.23616026
C	10.68556049	-3.74065521	-0.36905766
C	4.30788485	2.40976698	0.17509635
C	6.41970713	1.20577383	-0.07326930
C	9.97088726	-0.03056889	-0.13002156
C	10.68328164	-1.26858368	-0.19457683

C	12.81661786	-2.52034245	-0.31436598
C	6.43390868	3.64838276	-0.21474015
C	8.55207805	2.43503750	-0.06840902
C	10.68317438	1.19986167	-0.10098972
C	12.81785955	-0.04010945	-0.22347307
C	14.95755148	-1.28771759	-0.30055867
C	8.57125318	4.87014894	0.17488779
C	10.68282579	3.66583088	-0.07480497
C	12.81493609	2.42873377	-0.10835175
C	14.95007419	1.18484895	-0.14761213
C	17.08389061	-0.05795474	-0.34207508
C	3.57219232	1.22307137	-0.03715171
C	5.70884128	-0.02325597	-0.05893626
C	7.83855076	-1.26105595	-0.14162877
C	9.96905118	-2.49449061	-0.26706528
C	12.08382168	-3.72125853	-0.19265289
C	5.70047720	2.45586570	-0.04079588
C	7.83750237	1.20893916	-0.10324830
C	12.10195373	-1.26886734	-0.24927736
C	14.22017953	-2.47650977	-0.51821271
C	7.83330926	3.68417413	-0.03490236
C	9.97076618	2.43808202	-0.06327440
C	12.10333957	1.19896699	-0.13912743
C	14.23909536	-0.04211708	-0.22187256
C	16.36332331	-1.25802493	-0.17260059
C	9.96336523	4.91554323	-0.04429453
C	12.10092070	3.66781843	-0.10035076
C	14.23665882	2.42341510	-0.10171120
C	16.36571252	1.18824257	-0.23520852
C	18.46525986	0.00313867	-0.62221517
Br	17.26194373	-2.76498019	0.59157484
Br	15.00101211	-3.82761172	-1.62508563
Br	12.92057552	-5.24332086	0.60793357

Br	7.75707977	6.29152682	1.16295961
Br	5.59779586	5.10213281	-1.13949845
Br	3.48625076	3.82754610	1.16143543
Br	1.33900577	2.63627634	-1.15461467
Br	19.23678649	-1.34135041	-1.73786149
C	8.55032551	-0.02993889	-0.12159353
O	15.82941553	-0.47873984	2.47536094
H	16.66473968	-0.88561259	2.74240555
H	15.17472240	-1.21111888	2.57680818
O	14.02476070	-2.52538990	2.64433137
H	13.16458181	-2.09258300	2.76398610
H	14.02945689	-2.78794776	1.70520531

**g. Final**

C	2.18055496	1.17074008	-0.25157233
C	4.29833946	-0.04125892	-0.07414186
C	6.42971466	-1.27612195	-0.08712215
C	8.56038692	-2.50941802	-0.24290972
C	10.69433420	-3.74441710	-0.43833726
C	4.31364721	2.39567580	0.14833695
C	6.42766965	1.18913451	-0.07960330
C	9.98090953	-0.04516090	-0.10776888
C	10.69432464	-1.28003100	-0.18867929
C	12.82744634	-2.51262588	-0.44204098
C	6.44172567	3.63068131	-0.25072551
C	8.55945229	2.41904124	-0.07375179
C	10.69177315	1.18554194	-0.08705937
C	12.82538601	-0.04609792	-0.24524047
C	14.95866012	-1.28462280	-0.44787004
C	8.57524938	4.85558792	0.14805715
C	10.68969789	3.64996995	-0.08006890
C	12.82279182	2.41658798	-0.10800892
C	14.95784600	1.17761940	-0.19114251
C	17.09012455	-0.05623397	-0.44248723

C	3.57852665	1.20661374	-0.05917770
C	5.71674672	-0.03891673	-0.05805189
C	7.84891936	-1.27465385	-0.12932400
C	9.97892667	-2.50360150	-0.27982265
C	12.10090634	-3.71804420	-0.32700279
C	5.70843187	2.43749920	-0.06593175
C	7.84565587	1.19333553	-0.10161326
C	12.11128376	-1.27173651	-0.27932489
C	14.21385485	-2.45645534	-0.71702899
C	7.84002997	3.66695083	-0.05884643
C	9.97833630	2.42222949	-0.05842895
C	12.11178555	1.18742735	-0.13140939
C	14.24364872	-0.04454123	-0.28410098
C	16.36433035	-1.26085561	-0.33909238
C	9.97001262	4.89824561	-0.06636959
C	12.10801764	3.65373575	-0.10244530
C	14.24418246	2.41231115	-0.10978111
C	16.37335285	1.18331893	-0.27806370
C	18.47615400	0.00357933	-0.70868447
Br	17.24422054	-2.79671791	0.38881048
Br	14.95955011	-3.77885407	-1.87882223
Br	12.98807248	-5.23677918	0.44362261
Br	7.75486584	6.28074846	1.12275012
Br	5.60957671	5.07501634	-1.18954057
Br	3.49299097	3.81968591	1.12368988
Br	1.34832891	2.61484622	-1.19056666
Br	19.25663821	-1.31305876	-1.85689231
C	8.55969596	-0.04402712	-0.10579325
O	15.89677907	-0.45316281	2.63695168
H	16.71612164	-0.89230191	2.90442689
H	15.21009515	-1.14892085	2.72599352
O	13.75602794	-2.32350133	2.85294220
H	12.96390664	-1.93030581	3.24875161

H 13.45283273 -2.75317380 2.03523738

## 5) HOOH formation

### a. Initial

C	2.20544586	1.20544398	-0.24477432
C	4.32294924	-0.00142114	-0.06826068
C	6.45632818	-1.23065329	-0.08341932
C	8.58687837	-2.46159766	-0.18977642
C	10.70955425	-3.71951666	-0.35925421
C	4.33950857	2.43094208	0.17027391
C	6.45159573	1.23154864	-0.07187342
C	10.00164233	-0.00376248	-0.15177595
C	10.71288526	-1.23991232	-0.23111954
C	12.83018673	-2.48288541	-0.25730723
C	6.46462953	3.67001403	-0.23739113
C	8.58266594	2.46138143	-0.07176040
C	10.71449801	1.22511658	-0.11746608
C	12.84238148	-0.00948276	-0.22980241
C	14.94956976	-1.22981422	-0.01791444
C	8.60398081	4.89163859	0.16983874
C	10.71553631	3.68713718	-0.07679092
C	12.84717991	2.45518599	-0.10990263
C	14.98482162	1.22815673	-0.04723532
C	17.13213935	-0.00315641	-0.10195073
C	3.60367774	1.24397122	-0.04716061
C	5.74263429	0.00241704	-0.05564901
C	7.87436565	-1.23060192	-0.13652781
C	10.00587423	-2.47197570	-0.26212191
C	12.12125050	-3.68429547	-0.20741029
C	5.73328782	2.47683050	-0.04537432
C	7.87013126	1.23414231	-0.10453687
C	12.13061612	-1.24196456	-0.27615198
C	14.29546501	-2.48851537	-0.25129398
C	7.86338599	3.70858136	-0.04491941

C	10.00293755	2.45985343	-0.06586494
C	12.13859683	1.22042820	-0.15756177
C	14.27041805	-0.01669532	-0.11545869
C	16.34484794	-1.13803170	0.51167176
C	9.99814576	4.93213154	-0.04951842
C	12.13644773	3.68663673	-0.10451882
C	14.27410625	2.45186101	-0.08196823
C	16.41061557	1.23356908	-0.07450116
C	18.45691299	0.00587868	-0.51397661
Br	17.29472889	-2.91781152	0.67719040
Br	14.95776030	-3.19188438	-2.18801460
Br	13.07196963	-5.26573046	0.29070419
Br	7.78972598	6.31535975	1.14980161
Br	5.63046201	5.11536315	-1.16730618
Br	3.51373888	3.84922794	1.14856852
Br	1.37447299	2.64291318	-1.18753878
Br	19.11356802	-1.39835878	-1.62692072
C	8.58170120	0.00053518	-0.12654046
O	16.05035578	-0.77287324	1.87499072
O	17.28345756	-0.39906960	2.64347740
H	17.58800591	-1.29686758	2.89694292
H	14.17358878	-1.23803175	3.40705581
O	13.42293088	-1.78540997	3.12798684
H	12.74902525	-1.66733765	3.81112906
H	14.72511812	-3.31492255	0.31031540

**b. Transition State 1**

C	2.20262328	1.21825120	-0.24411619
C	4.31991134	0.01256704	-0.06220861
C	6.45313361	-1.21705078	-0.08605780
C	8.58217994	-2.45126232	-0.20974475
C	10.70520727	-3.70159526	-0.38406319
C	4.33735985	2.44490269	0.16950535
C	6.44947102	1.24469177	-0.06641723



C	9.99944411	0.00993968	-0.13764335
C	10.70954073	-1.22577949	-0.22129757
C	12.81841269	-2.46950024	-0.29313510
C	6.46276606	3.68182806	-0.24198349
C	8.58069376	2.47377659	-0.06661551
C	10.71260235	1.23749226	-0.10807713
C	12.84195897	0.00445082	-0.26338701
C	14.97475835	-1.20609496	-0.19441969
C	8.60087796	4.90395447	0.16903433
C	10.71284166	3.70076737	-0.07201307
C	12.84452652	2.46866575	-0.11634962
C	14.97986054	1.24342080	-0.14511827
C	17.11273382	0.00374145	-0.24540200
C	3.60000759	1.25906762	-0.04381406
C	5.73975650	0.01647544	-0.04960312
C	7.87144450	-1.21903634	-0.13503450
C	10.00089614	-2.45725053	-0.26239877
C	12.11835888	-3.66807592	-0.23446895
C	5.73083448	2.48975743	-0.04603275
C	7.86809751	1.24627333	-0.09723038
C	12.12481227	-1.22823192	-0.29295549
C	14.28099505	-2.48021747	-0.33265085
C	7.86099414	3.72097883	-0.04534296
C	10.00094801	2.47268760	-0.05982952
C	12.13602908	1.23323561	-0.16250065
C	14.27131590	0.01121522	-0.24688662
C	16.35807707	-1.17584883	0.07547998
C	9.99492986	4.94560287	-0.04758954
C	12.13286034	3.70234995	-0.09997788
C	14.26690335	2.47173676	-0.10938484
C	16.39951882	1.24469376	-0.16864729
C	18.46657406	0.03943856	-0.59800189
Br	17.27045435	-2.79178768	0.55311566

Br	14.95013259	-3.28473222	-2.14687653
Br	13.05820495	-5.24692800	0.28271705
Br	7.78183984	6.32893649	1.14309299
Br	5.62948985	5.12448192	-1.17673255
Br	3.51163752	3.86821751	1.14072010
Br	1.36975199	2.65569272	-1.18604790
Br	19.15497832	-1.31320301	-1.75972419
C	8.57959123	0.01180051	-0.11471531
O	16.01598657	-0.57415616	2.20311867
O	17.25586407	-0.42987403	2.83450198
H	17.46069063	-1.35232701	3.09955346
H	14.59175196	-1.58507032	2.73267280
O	13.77821209	-2.13837429	2.80456048
H	13.12367814	-1.55789613	3.22084820
H	14.68666515	-3.23593418	0.34366881

**c. Transition State 2**

C	2.19660762	1.22225925	-0.24160300
C	4.31298189	0.01516029	-0.05795235
C	6.44516710	-1.21465135	-0.08883095
C	8.57314135	-2.44898674	-0.22811407
C	10.69654616	-3.69595272	-0.41747841
C	4.33143826	2.44918971	0.16809913
C	6.44293507	1.24709821	-0.06302467
C	9.99121949	0.01420503	-0.15539399
C	10.69899958	-1.21986526	-0.26703476
C	12.80179102	-2.45975547	-0.41473812
C	6.45728208	3.68460282	-0.24036297
C	8.57447867	2.47564202	-0.06334109
C	10.70614409	1.24036701	-0.11975573
C	12.83486338	0.01117347	-0.32246634
C	14.97872253	-1.19573963	-0.28386266
C	8.59482333	4.90821704	0.16774775
C	10.70622231	3.70398520	-0.06991289

C	12.83711034	2.47086911	-0.12393435
C	14.96979750	1.24759195	-0.19439587
C	17.10452380	0.00771943	-0.29805427
C	3.59374689	1.26277489	-0.04157759
C	5.73282199	0.01944162	-0.04621149
C	7.86301566	-1.21655864	-0.14011918
C	9.99015471	-2.45327656	-0.28418785
C	12.11322699	-3.65706967	-0.30122473
C	5.72489289	2.49287011	-0.04556562
C	7.86108278	1.24829602	-0.09361434
C	12.11043689	-1.21824161	-0.39422259
C	14.26652509	-2.47191956	-0.41400772
C	7.85544264	3.72375507	-0.04333929
C	9.99467882	2.47550601	-0.05984713
C	12.12822334	1.23718735	-0.18688511
C	14.26213176	0.02414768	-0.30925867
C	16.35353728	-1.18272511	-0.09594226
C	9.98870382	4.94965208	-0.04690087
C	12.12521572	3.70597190	-0.09730179
C	14.25694391	2.47729376	-0.12548508
C	16.38901489	1.24681787	-0.22010931
C	18.46897699	0.04623539	-0.62537830
Br	17.23122632	-2.76175388	0.52399618
Br	14.94250487	-3.37758007	-2.10573845
Br	13.04793852	-5.21474240	0.28491028
Br	7.77520386	6.33303707	1.14046566
Br	5.62508551	5.12627571	-1.17689598
Br	3.50722955	3.87253020	1.13947069
Br	1.36393257	2.65996471	-1.18327649
Br	19.17312570	-1.31080290	-1.77695187
C	8.57210609	0.01307869	-0.11580159
O	15.85415251	-0.30896074	2.40831416
O	17.10132460	-0.47171748	3.00530244

H	17.19220454	-1.44888493	3.09302056
H	14.76520553	-1.62708924	2.56331907
O	14.08967459	-2.35470824	2.63508850
H	13.24072588	-1.90469276	2.54692838
H	14.60277132	-3.14658889	0.38944541

**d. Transition State 3**

C	2.19376327	1.22068940	-0.23890945
C	4.30908993	0.01228339	-0.05535466
C	6.43940910	-1.21878345	-0.08822581
C	8.56607417	-2.45389839	-0.23210213
C	10.69293809	-3.69947988	-0.42704720
C	4.32844705	2.44791289	0.16886805
C	6.43874520	1.24443015	-0.06106052
C	9.98452047	0.01025054	-0.14729450
C	10.68940870	-1.22429818	-0.26270088
C	12.78824470	-2.45874203	-0.47377381
C	6.45429939	3.68296848	-0.23811260
C	8.57029481	2.47291825	-0.05962433
C	10.70004828	1.23680135	-0.11715870
C	12.82462838	0.01053916	-0.37136464
C	14.97217606	-1.18968745	-0.43973265
C	8.59182422	4.90702626	0.16833499
C	10.70208504	3.70167291	-0.06767745
C	12.83058701	2.46720530	-0.13330035
C	14.96116225	1.24545480	-0.24611544
C	17.09812858	0.00800447	-0.38766699
C	3.59061575	1.26086248	-0.03892034
C	5.72850287	0.01656469	-0.04378540
C	7.85698133	-1.22057827	-0.13550729
C	9.98298695	-2.45868808	-0.28353016
C	12.11012711	-3.65878985	-0.32490168
C	5.72150110	2.49108347	-0.04427337
C	7.85631875	1.24577600	-0.09070995

C	12.09678840	-1.22046692	-0.41924110
C	14.25205513	-2.46362165	-0.49536459
C	7.85217556	3.72204220	-0.04072835
C	9.99023905	2.47304083	-0.05607465
C	12.12064560	1.23489210	-0.20210684
C	14.25173467	0.02860726	-0.40763357
C	16.34621126	-1.18789060	-0.24491603
C	9.98530014	4.94825705	-0.04544246
C	12.12038905	3.70335493	-0.09624193
C	14.25015723	2.47388037	-0.14041917
C	16.38094258	1.24198181	-0.26113535
C	18.47237174	0.04537698	-0.66362204
Br	17.21513746	-2.76045023	0.41043465
Br	14.93487716	-3.47042792	-2.06460038
Br	13.04985459	-5.19982172	0.29587408
Br	7.77186184	6.33400847	1.13898348
Br	5.62298950	5.12481559	-1.17637798
Br	3.50432137	3.87307137	1.13920180
Br	1.36246082	2.65950382	-1.18194647
Br	19.21109947	-1.29443442	-1.81623459
C	8.56613641	0.00932653	-0.10909202
O	15.73402294	-0.37501435	2.42251679
O	17.00060668	-0.52407995	3.00648111
H	17.12417519	-1.49915912	3.07097146
H	14.94528323	-1.63183016	2.37803107
O	14.30602661	-2.44451849	2.27473360
H	13.41517679	-2.07060801	2.22693213
H	14.48070801	-2.87616561	0.58525528

**e. Transition State 4**

C	2.19380071	1.22048607	-0.23711279
C	4.30913345	0.01204988	-0.05477139
C	6.43932295	-1.22054251	-0.08871253
C	8.56632836	-2.45634304	-0.23233587

C	10.69587977	-3.70232479	-0.42891622
C	4.32845992	2.44791114	0.16853444
C	6.43914561	1.24377919	-0.06041717
C	9.98519733	0.00896957	-0.14709420
C	10.69173639	-1.22710034	-0.25756268
C	12.80405739	-2.46465817	-0.47261307
C	6.45434631	3.68254521	-0.23608337
C	8.57039819	2.47261772	-0.05907121
C	10.70038140	1.23693387	-0.11727914
C	12.82481345	0.00845616	-0.36353706
C	14.96272562	-1.21591144	-0.44368747
C	8.59181283	4.90704674	0.16817234
C	10.70230020	3.70141052	-0.06733363
C	12.83017618	2.46666267	-0.13316013
C	14.96077698	1.23877802	-0.23975696
C	17.09511530	0.00081735	-0.38918339
C	3.59134637	1.25968801	-0.03808205
C	5.72857484	0.01584386	-0.04465375
C	7.85727696	-1.22179153	-0.13475774
C	9.98372950	-2.45940060	-0.28533315
C	12.10702339	-3.66808422	-0.33293527
C	5.72233618	2.48970999	-0.04325875
C	7.85661981	1.24538747	-0.09073370
C	12.10220787	-1.22106106	-0.40110394
C	14.23758518	-2.45532374	-0.57672147
C	7.85282297	3.72068777	-0.04007080
C	9.99012727	2.47350953	-0.05617192
C	12.11920596	1.23659349	-0.20303048
C	14.24708133	0.02101203	-0.38836097
C	16.34986652	-1.19433420	-0.25382772
C	9.98575669	4.94731129	-0.04484332
C	12.12016893	3.70369094	-0.09543918
C	14.25048488	2.47116263	-0.13900029

C	16.37986659	1.23872780	-0.26196923
C	18.47314789	0.04128764	-0.66164107
Br	17.21561654	-2.76665450	0.41120733
Br	14.92724944	-3.56327576	-2.02346231
Br	13.04876293	-5.20541451	0.29923238
Br	7.77122962	6.33534952	1.13898164
Br	5.62268638	5.12518588	-1.17622273
Br	3.50386684	3.87408155	1.13943365
Br	1.36221876	2.66000178	-1.18199289
Br	19.21172603	-1.29625080	-1.81669557
C	8.56663743	0.00826509	-0.10928352
O	15.63820842	-0.45104697	2.43355077
O	16.97218721	-0.53936636	3.00673927
H	17.13604779	-1.50399000	3.06731045
H	15.09042589	-1.48242066	2.37633320
O	14.31701872	-2.51716991	2.10779642
H	13.42983208	-2.11368154	2.20298500
H	14.41565367	-2.76736877	0.96038490

**f. Transition State 5**

C	2.19170442	1.20291872	-0.23404368
C	4.30821858	-0.00951375	-0.06390365
C	6.43844039	-1.24661310	-0.08871780
C	8.56657580	-2.48589430	-0.23926755
C	10.69924638	-3.72973814	-0.43257579
C	4.32746726	2.42701034	0.16792995
C	6.43831706	1.22146906	-0.06978744
C	9.98659932	-0.01829071	-0.11645351
C	10.69683549	-1.25791563	-0.19497883
C	12.82562517	-2.49254025	-0.42599542
C	6.45235012	3.66355735	-0.23191997
C	8.56886126	2.45069341	-0.06555601
C	10.69875273	1.21426004	-0.09336163
C	12.82853646	-0.02043297	-0.24459960

C	14.96059506	-1.26262248	-0.41540621
C	8.58962125	4.88720681	0.16593648
C	10.70057931	3.68149972	-0.07175087
C	12.83004965	2.44513724	-0.10803445
C	14.96203515	1.20309307	-0.18675305
C	17.09371373	-0.03767346	-0.42489612
C	3.58933006	1.24042460	-0.04189226
C	5.72731897	-0.00711886	-0.05408920
C	7.85727421	-1.24744373	-0.13349279
C	9.98470211	-2.48551994	-0.27774896
C	12.10676590	-3.70221331	-0.32610711
C	5.72041156	2.47081278	-0.04605806
C	7.85527895	1.22342238	-0.09649076
C	12.11412894	-1.24926683	-0.27754947
C	14.22311522	-2.44702583	-0.65807834
C	7.85049610	3.70082347	-0.04263662
C	9.98806022	2.45342875	-0.05734176
C	12.11802405	1.21627572	-0.13975442
C	14.24685789	-0.02043324	-0.27389051
C	16.36474979	-1.24075123	-0.31428797
C	9.98260604	4.93056423	-0.04883384
C	12.11814755	3.68376865	-0.09647559
C	14.25095412	2.44131310	-0.11159410
C	16.37840669	1.20577436	-0.26886346
C	18.47847457	0.01586726	-0.69199398
Br	17.22459600	-2.79785088	0.39932767
Br	14.91962172	-3.65612361	-1.98232423
Br	13.02835909	-5.22661687	0.36922919
Br	7.76980888	6.31443093	1.13980962
Br	5.61807083	5.11083639	-1.16430053
Br	3.50565415	3.85142356	1.14461594
Br	1.35925366	2.64946808	-1.16916255
Br	19.23602890	-1.31001637	-1.84131816



C	8.56657251	-0.01614034	-0.10806282
O	15.76039964	-0.50483679	2.43609415
O	17.01960958	-0.55667187	3.20402315
H	17.45665539	-1.31454955	2.75982540
H	15.20593555	-1.21936071	2.84623393
O	13.87098304	-2.41569402	2.65891257
H	13.04384812	-1.90731123	2.68845826
H	13.98822332	-2.62919675	1.71387430

**g. Final**

C	2.19031569	1.19075422	-0.24024271
C	4.30793819	-0.02255185	-0.06903930
C	6.43857857	-1.25884989	-0.08633079
C	8.56675902	-2.49415971	-0.23788127
C	10.69847793	-3.72897696	-0.43590675
C	4.32548151	2.41318458	0.16082505
C	6.43770430	1.20869010	-0.07500995
C	9.98817579	-0.02718035	-0.10573189
C	10.69889706	-1.26408771	-0.18081035
C	12.82923218	-2.49581160	-0.43758186
C	6.45117063	3.65059048	-0.23901876
C	8.56874467	2.43822360	-0.06945962
C	10.70057479	1.20440672	-0.08703548
C	12.83208666	-0.02955558	-0.24121051
C	14.96385301	-1.27442118	-0.46460539
C	8.58728477	4.87392342	0.15898186
C	10.69992438	3.66999656	-0.07562218
C	12.83130617	2.43421040	-0.10490106
C	14.96468131	1.19004949	-0.18583461
C	17.09616739	-0.04528470	-0.45380354
C	3.58813625	1.22623510	-0.04883265
C	5.72676551	-0.01991880	-0.05625474
C	7.85763873	-1.25762208	-0.12828719
C	9.98436833	-2.48859186	-0.27359323

C	12.10487575	-3.70327326	-0.32241868
C	5.71893164	2.45768133	-0.05429349
C	7.85503184	1.21164642	-0.09854830
C	12.11594744	-1.25482649	-0.27217534
C	14.20864526	-2.43872792	-0.73943521
C	7.84940083	3.68681076	-0.04947618
C	9.98780560	2.44227216	-0.05736989
C	12.12057866	1.20528049	-0.13039963
C	14.25030408	-0.03313690	-0.28152196
C	16.37224660	-1.25434284	-0.37780897
C	9.98099298	4.91844305	-0.05595811
C	12.11772296	3.67198072	-0.09843721
C	14.25251089	2.42821650	-0.10658226
C	16.38095729	1.19595776	-0.27419285
C	18.48078669	0.02259797	-0.72677323
Br	17.27347033	-2.82349477	0.23815084
Br	14.91199401	-3.74897146	-1.94118616
Br	12.99434554	-5.22440457	0.43281365
Br	7.76740354	6.29871923	1.13637209
Br	5.61760040	5.09579027	-1.17490758
Br	3.50496742	3.83658380	1.13920599
Br	1.35869882	2.63598707	-1.17735366
Br	19.26988883	-1.24785492	-1.91812388
C	8.56771283	-0.02646082	-0.10415725
O	15.95227447	-0.84618932	2.42185872
O	17.15581315	-0.46065135	3.18817142
H	17.50285400	-1.34509691	3.41134297
H	15.24045972	-0.81788396	3.09880210
O	13.50074600	-1.70849571	3.20683534
H	12.62275754	-1.74076291	3.61271662
H	13.42261420	-2.22869030	2.38934399

**7) OO Dissociation**  
**a. Initial**

C	2.15501398	1.19905925	-0.16285304
C	4.27504845	-0.01352448	-0.05457144
C	6.40514035	-1.24229803	-0.09243062
C	8.53535844	-2.46905107	-0.12572585
C	10.66031042	-3.71738447	-0.08749865
C	4.29166525	2.41758345	0.23138057
C	6.40364790	1.22223122	-0.06020036
C	9.95934084	-0.01317448	-0.09875977
C	10.67212936	-1.25054165	-0.08470328
C	12.76549442	-2.51280024	0.10828953
C	6.41736277	3.65993566	-0.17396005
C	8.54015699	2.44900651	-0.06096669
C	10.67402484	1.21194750	-0.08938096
C	12.81333849	-0.03748749	-0.10652768
C	14.98016171	-1.24023328	0.09352271
C	8.55320029	4.87649314	0.23307552
C	10.66755127	3.67979302	-0.05765945
C	12.80230801	2.44059813	-0.10396319
C	14.93617211	1.20680747	-0.08512749
C	17.08091996	-0.01545258	-0.09860217
C	3.55633869	1.23133707	0.00463595
C	5.69360098	-0.00746192	-0.05799734
C	7.82344715	-1.23590256	-0.11826459
C	9.95213883	-2.47354209	-0.09014023
C	12.04503125	-3.69080873	0.22567039
C	5.68366709	2.46667326	-0.00292842
C	7.82343980	1.22511690	-0.10014602
C	12.08979026	-1.26764128	-0.07642083
C	14.24486346	-2.52324909	0.27062898
C	7.81973591	3.69245807	-0.00278142
C	9.96001236	2.44919986	-0.06052889
C	12.09987271	1.19970351	-0.10413476
C	14.24021131	-0.02903416	-0.08001627
C	16.36368623	-1.20879719	0.19063670
C	9.94678147	4.92417153	0.00465858
C	12.08677996	3.67912907	-0.09721035
C	14.22061816	2.44424186	-0.09689584
C	16.35635128	1.22031408	-0.09004217
C	18.46576353	0.02024216	-0.34244222
Br	17.35717312	-2.61875642	1.01927921
Br	14.98361866	-3.83432323	-1.09102377
Br	12.75747830	-5.24570570	1.08386686
Br	7.74751185	6.26410670	1.27310312
Br	5.56910659	5.13470801	-1.04910868
Br	3.49042325	3.81131490	1.26757931
Br	1.30301086	2.67394998	-1.03448426

Br	19.27908490	-1.35471217	-1.39196930
C	8.53713085	-0.00947426	-0.11025363
O	14.53103608	-3.01188659	1.68831309
O	14.05684462	-2.06597596	2.51234752

**b. Transition State 1**

C	2.15417277	1.19281022	-0.17835906
C	4.27243797	-0.01970357	-0.05978675
C	6.40131898	-1.24881410	-0.08957308
C	8.53093504	-2.47475904	-0.12209288
C	10.65597703	-3.72249363	-0.12672439
C	4.28914200	2.41234453	0.22051540
C	6.40104035	1.21619948	-0.06313749
C	9.95603553	-0.02018302	-0.09522010
C	10.66827822	-1.25796122	-0.08734820
C	12.76185594	-2.52414278	0.07658325
C	6.41621825	3.65515259	-0.17848311
C	8.53764130	2.44328008	-0.06287036
C	10.67049767	1.20485737	-0.08778395
C	12.80814858	-0.04673303	-0.10262725
C	14.97532794	-1.24956935	0.08970688
C	8.55252349	4.87184352	0.22267853
C	10.66530643	3.67281713	-0.06409801
C	12.79886040	2.43332770	-0.10155355
C	14.93135029	1.19972576	-0.07765890
C	17.07341593	-0.01958266	-0.11977897
C	3.55460278	1.22579337	-0.00665920
C	5.69044895	-0.01346772	-0.05979015
C	7.81970637	-1.24178169	-0.11275042
C	9.94780888	-2.47998639	-0.09578452
C	12.04685665	-3.70867876	0.15493406
C	5.68174271	2.46178610	-0.00914918
C	7.82079645	1.21964306	-0.09989714
C	12.08472003	-1.27662727	-0.08286982
C	14.23916999	-2.53541490	0.25041732
C	7.81808703	3.68763006	-0.00740810
C	9.95710428	2.44258077	-0.06241297
C	12.09615605	1.19172190	-0.10065846
C	14.23506099	-0.03703711	-0.07399572
C	16.36091747	-1.21719186	0.16596234
C	9.94571471	4.91860121	-0.00796369
C	12.08443588	3.67251863	-0.10009313
C	14.21700338	2.43687418	-0.09180120
C	16.35044201	1.21508730	-0.08882982
C	18.45079006	0.02651287	-0.40428889
Br	17.36707141	-2.63967729	0.95463080
Br	14.98528105	-3.81348671	-1.14396335

Br	12.77142474	-5.29151455	0.94774158
Br	7.75031051	6.26409725	1.25937217
Br	5.56956275	5.12990699	-1.05574830
Br	3.48262976	3.80754953	1.25031809
Br	1.30346954	2.66367021	-1.05795467
Br	19.22316945	-1.32421937	-1.51123110
C	8.53408918	-0.01511582	-0.10683205
O	14.51878320	-3.02016131	1.68041084
O	13.71833509	-2.32204641	2.49222241

**c. Transition State 2**

C	2.15282030	1.19233579	-0.17508499
C	4.27047479	-0.02047380	-0.05803112
C	6.39816847	-1.25002173	-0.09067492
C	8.52684303	-2.47554225	-0.13472434
C	10.65307474	-3.72288593	-0.13705760
C	4.28753790	2.41168179	0.22417577
C	6.39885750	1.21573973	-0.06201900
C	9.95187163	-0.02090019	-0.09802200
C	10.66138265	-1.25909431	-0.08509228
C	12.74710259	-2.52427583	0.09942583
C	6.41464432	3.65497024	-0.17642502
C	8.53556638	2.44281701	-0.06331394
C	10.66782642	1.20346016	-0.08900901
C	12.80383955	-0.05111090	-0.09147206
C	14.97338019	-1.25112802	0.08956156
C	8.55116297	4.87117653	0.22553438
C	10.66340821	3.67189215	-0.06378895
C	12.79611342	2.43154901	-0.10115368
C	14.92722830	1.19794179	-0.08011139
C	17.06733987	-0.01953275	-0.17159411
C	3.55314548	1.22535375	-0.00306814
C	5.68815041	-0.01434776	-0.05855685
C	7.81658398	-1.24247725	-0.11758019
C	9.94232636	-2.48097512	-0.10051807
C	12.03867012	-3.71782833	0.15276656
C	5.68011954	2.46140762	-0.00702778
C	7.81837843	1.21938287	-0.10071885
C	12.07588074	-1.27925595	-0.07186561
C	14.23291517	-2.53777850	0.25244956
C	7.81651410	3.68717762	-0.00637673
C	9.95512900	2.44143105	-0.06349679
C	12.09347510	1.18903666	-0.09840069
C	14.23125860	-0.04020077	-0.06635422
C	16.35972368	-1.21896657	0.13020424
C	9.94416313	4.91796468	-0.00577225
C	12.08253131	3.67148252	-0.09976193

C	14.21384944	2.43571930	-0.09125604
C	16.34477187	1.21405436	-0.10650135
C	18.44566222	0.03495654	-0.45013335
Br	17.36770828	-2.66681230	0.86952672
Br	14.91625764	-3.76422858	-1.22627096
Br	12.76223241	-5.33682165	0.87770404
Br	7.74926457	6.26166748	1.26455529
Br	5.56676561	5.13035512	-1.05129297
Br	3.48231204	3.80527426	1.25717243
Br	1.30190653	2.66435746	-1.05240690
Br	19.20332498	-1.28290372	-1.60780948
C	8.53082381	-0.01544560	-0.10980041
O	14.45114632	-3.02750977	1.66005460
O	13.43032997	-2.44284009	2.33831812

**d. Transition State 3**

C	2.15322004	1.19215274	-0.17536782
C	4.27131083	-0.02122794	-0.05833924
C	6.39967156	-1.25105025	-0.09069913
C	8.53256640	-2.47553172	-0.14026334
C	10.66551929	-3.72407805	-0.12879949
C	4.28777697	2.41142404	0.22460811
C	6.39997871	1.21531168	-0.06220790
C	9.95392319	-0.02304380	-0.10271056
C	10.66384433	-1.26070463	-0.07820264
C	12.75295015	-2.51405078	0.24742554
C	6.41489087	3.65468164	-0.17666138
C	8.53613529	2.44214258	-0.06363404
C	10.67006558	1.20246492	-0.09069719
C	12.80446372	-0.05578239	-0.08217659
C	14.98372127	-1.24671168	0.08817261
C	8.55181162	4.87044233	0.22623178
C	10.66405749	3.67086599	-0.06437600
C	12.79808061	2.43061165	-0.10425858
C	14.93035513	1.19768292	-0.08229422
C	17.06986018	-0.01873232	-0.17185895
C	3.55354931	1.22474878	-0.00302381
C	5.68918019	-0.01554551	-0.05873698
C	7.81967297	-1.24343419	-0.11877594
C	9.94511715	-2.48128516	-0.10169701
C	12.03651400	-3.72989938	0.19171842
C	5.68084272	2.46102488	-0.00681802
C	7.81907942	1.21853519	-0.10196202
C	12.07766593	-1.28029046	-0.03582536
C	14.26164121	-2.53928703	0.27928396
C	7.81697996	3.68622216	-0.00660030
C	9.95613320	2.44064102	-0.06341249

C	12.09516821	1.18702470	-0.10149240
C	14.23664126	-0.04242684	-0.06338634
C	16.36970822	-1.21616589	0.13025561
C	9.94480839	4.91715560	-0.00607800
C	12.08398743	3.67015880	-0.10085927
C	14.21546174	2.43546425	-0.09215109
C	16.34631794	1.21287900	-0.11203569
C	18.45161421	0.03550619	-0.45519482
Br	17.37109098	-2.67400843	0.85595391
Br	14.87087788	-3.74018745	-1.26430851
Br	12.76158647	-5.35965557	0.88039531
Br	7.75020273	6.26044674	1.26469157
Br	5.56702783	5.13002086	-1.05075519
Br	3.48322386	3.80419111	1.25786911
Br	1.30229326	2.66386540	-1.05202833
Br	19.19671202	-1.27051562	-1.62794152
C	8.53226277	-0.01653514	-0.11284493
O	14.49266544	-3.03034551	1.62300786
O	13.30215431	-2.47320534	2.18375754

**e. Transition State 4**

C	2.15370999	1.19246726	-0.17518940
C	4.27170576	-0.02132334	-0.05809596
C	6.40058769	-1.25147913	-0.09022212
C	8.53912622	-2.47487607	-0.14188070
C	10.67641087	-3.72612015	-0.13892386
C	4.28798662	2.41145271	0.22481456
C	6.40062978	1.21570516	-0.06213438
C	9.95470553	-0.02240359	-0.10542502
C	10.66789653	-1.25907561	-0.06874720
C	12.77494062	-2.50289871	0.40838203
C	6.41484456	3.65483472	-0.17661667
C	8.53646558	2.44261033	-0.06374789
C	10.67088895	1.20270146	-0.09134008
C	12.80031553	-0.05913439	-0.07367314
C	14.98825875	-1.24486710	0.08359950
C	8.55217599	4.87081834	0.22652191
C	10.66426274	3.67087931	-0.06448232
C	12.79911328	2.43051080	-0.10652247
C	14.93166786	1.19555299	-0.08327826
C	17.07023149	-0.01864410	-0.17157868
C	3.55367647	1.22492492	-0.00323425
C	5.68980108	-0.01544190	-0.05874091
C	7.82142018	-1.24260371	-0.11772659
C	9.94614912	-2.48054756	-0.10514605
C	12.02837468	-3.74625414	0.20978492
C	5.68110444	2.46170201	-0.00647540

C	7.81901110	1.21916605	-0.10257408
C	12.07556752	-1.27009402	0.00998915
C	14.28697650	-2.54637595	0.27625889
C	7.81718801	3.68675453	-0.00666308
C	9.95595105	2.44211320	-0.06295335
C	12.09372838	1.18795597	-0.10494366
C	14.23985996	-0.04500438	-0.05947357
C	16.37396753	-1.21352616	0.12924147
C	9.94456387	4.91753317	-0.00616881
C	12.08446793	3.67072340	-0.10118364
C	14.21579298	2.43528436	-0.09282838
C	16.34723435	1.21051065	-0.11641550
C	18.45529171	0.03207277	-0.46202656
Br	17.37000248	-2.67552458	0.85578667
Br	14.85983067	-3.74020831	-1.26608215
Br	12.75762814	-5.36483972	0.89054691
Br	7.75010865	6.26068207	1.26459786
Br	5.56698188	5.13004395	-1.05078572
Br	3.48320674	3.80444410	1.25808656
Br	1.30228152	2.66415456	-1.05240320
Br	19.19445734	-1.27118848	-1.63630886
C	8.53226372	-0.01646247	-0.11472131
O	14.52197095	-3.02367112	1.61095075
O	13.19387192	-2.45964855	2.03097464

**f. Transition State 5**

C	2.15467914	1.19309904	-0.17519711
C	4.27458679	-0.02054713	-0.05881507
C	6.40601706	-1.25097442	-0.09020185
C	8.54949786	-2.47273327	-0.14098037
C	10.69023304	-3.72823620	-0.14815978
C	4.28947905	2.41170631	0.22483752
C	6.40322602	1.21617514	-0.06230492
C	9.96050280	-0.01971372	-0.10440895
C	10.67909137	-1.25374520	-0.05760298
C	12.79908325	-2.49259753	0.50594331
C	6.41604379	3.65517012	-0.17675005
C	8.53872316	2.44387370	-0.06357192
C	10.67557516	1.20619223	-0.09126617
C	12.80826710	-0.05430197	-0.06367546
C	15.00065260	-1.25033392	0.07445847
C	8.55318563	4.87185141	0.22601427
C	10.66653749	3.67259419	-0.06404537
C	12.80318377	2.43255124	-0.10909547
C	14.94205808	1.19604109	-0.08740382
C	17.08653967	-0.01811956	-0.15440866
C	3.55553783	1.22513991	-0.00343615



C	5.69306745	-0.01483517	-0.05913172
C	7.82761647	-1.24125746	-0.11732335
C	9.95922077	-2.47787749	-0.10480410
C	12.03585768	-3.75121921	0.24377635
C	5.68272575	2.46169190	-0.00647132
C	7.82199481	1.22001426	-0.10339075
C	12.08563068	-1.25795287	0.04532290
C	14.31399480	-2.55724270	0.31777206
C	7.81854675	3.68741556	-0.00639388
C	9.95882311	2.44420464	-0.06317127
C	12.09787852	1.19299471	-0.10592515
C	14.24945221	-0.04675009	-0.06350342
C	16.38326761	-1.21403048	0.12681284
C	9.94594172	4.91864777	-0.00522885
C	12.08696044	3.67170172	-0.10206942
C	14.22264872	2.43562536	-0.09517885
C	16.35949672	1.21481893	-0.11238025
C	18.46188102	0.02892843	-0.46108177
Br	17.37437202	-2.67894088	0.84290661
Br	14.82647360	-3.74179511	-1.33963215
Br	12.75709888	-5.36028635	0.90552647
Br	7.75036773	6.26157722	1.26313019
Br	5.56739957	5.13005276	-1.05043101
Br	3.48400607	3.80395529	1.25686414
Br	1.30336270	2.66467908	-1.05133394
Br	19.19358311	-1.26843055	-1.64067290
C	8.53762710	-0.01480894	-0.11588497
O	14.66948857	-3.08276181	1.50992823
O	12.91593231	-2.41794280	1.96785135

**g. Final**

C	2.15175506	1.19908473	-0.16870071
C	4.27216336	-0.01217945	-0.05800285
C	6.40543511	-1.24479611	-0.09654029
C	8.53887527	-2.48177415	-0.18850967
C	10.66576026	-3.72918738	-0.32079496
C	4.28820167	2.41711409	0.23600652
C	6.39996604	1.21971898	-0.05948625
C	9.95481905	-0.01812715	-0.07314912
C	10.67295118	-1.25191014	-0.00637671
C	12.77640288	-2.46111055	0.42948493
C	6.41267104	3.65946448	-0.17312211
C	8.53363269	2.44792580	-0.06171279
C	10.66426401	1.21231244	-0.07621444
C	12.79773563	-0.01403171	-0.02734902
C	14.95887459	-1.24682220	-0.08776670
C	8.54882692	4.87635306	0.23285355

C	10.66158971	3.67965825	-0.06114565
C	12.79715921	2.44775420	-0.10491910
C	14.93162898	1.20837370	-0.15426921
C	17.05664047	-0.01918196	-0.48907323
C	3.55292252	1.23284280	0.00280057
C	5.69157094	-0.00940691	-0.05756090
C	7.82515662	-1.24560977	-0.11994002
C	9.96066278	-2.49951702	-0.11008403
C	12.08220920	-3.76835412	0.16972420
C	5.67968483	2.46608383	-0.00024248
C	7.81985261	1.22049703	-0.09966003
C	12.07594601	-1.22062155	0.08350551
C	14.27151589	-2.36402337	0.62883967
C	7.81429402	3.69313096	-0.00258621
C	9.95140905	2.44980469	-0.06033600
C	12.08566924	1.21755818	-0.08299484
C	14.22957158	-0.01353285	-0.08990385
C	16.35616291	-1.24091193	-0.30492028
C	9.94116678	4.92557894	-0.00010151
C	12.08176044	3.68295866	-0.10056226
C	14.21793116	2.44563616	-0.11010282
C	16.35111454	1.21155002	-0.26202352
C	18.45537176	0.10081701	-0.80579702
Br	17.27193140	-2.89437550	-0.22286314
Br	14.14023189	-2.34648582	-2.48120934
Br	13.18597564	-5.35701196	-0.04091895
Br	7.74506525	6.26492855	1.26709259
Br	5.56446967	5.12888882	-1.04948152
Br	3.48739857	3.80623371	1.27136649
Br	1.30489188	2.67033941	-1.04334949
Br	19.20491726	-1.00687437	-2.15016008
C	8.53364640	-0.01501580	-0.10291011
O	14.82620678	-3.04637635	1.46996824
O	12.12474455	-3.23360134	1.47974091

### ER Mechanism – ZU Iodine

#### 1) OOH formation

##### a. Initial

C	2.16313746	1.17840910	-0.21211030
C	4.28170337	-0.03662910	-0.07111098
C	6.41209585	-1.26987339	-0.08408074
C	8.54512239	-2.51025699	-0.09871992

C	10.67752318	-3.75892948	-0.08223305
C	4.29742856	2.39889819	0.19001241
C	6.41011578	1.19690406	-0.07541473
C	9.96421306	-0.04411600	-0.08514049
C	10.67655155	-1.28242138	-0.07063403
C	12.78634567	-2.53733594	0.00985608
C	6.42386072	3.64029311	-0.20936117
C	8.54427146	2.42478307	-0.07186405
C	10.67568494	1.18550048	-0.08535109
C	12.81119679	-0.06143495	-0.11082411
C	14.95928672	-1.27783554	0.03022773
C	8.56071603	4.85912539	0.18652240
C	10.67355246	3.65400317	-0.07869832
C	12.80660676	2.41658185	-0.10194393
C	14.93929884	1.17973506	-0.06454967
C	17.07798599	-0.06384362	-0.07015954
C	3.56307006	1.21131351	-0.03033956
C	5.70012718	-0.03273646	-0.06354337
C	7.83316277	-1.27233950	-0.10057152
C	9.96336192	-2.51024603	-0.07082309
C	12.08033245	-3.72244940	0.13353238
C	5.69072624	2.44511570	-0.03549041
C	7.82935348	1.19891277	-0.10546488
C	12.09074614	-1.29229528	-0.08934352
C	14.24303666	-2.54642437	-0.08701109
C	7.82519477	3.67260505	-0.03111443
C	9.96327342	2.42416415	-0.06601668
C	12.10036955	1.17650873	-0.09980108
C	14.23601086	-0.04990695	-0.08349377
C	16.34033126	-1.25548404	0.16351681
C	9.95447649	4.90233664	-0.03943434
C	12.09284774	3.65564822	-0.10815909
C	14.22673004	2.41731397	-0.08355860

C	16.35857437	1.18110931	-0.06469854
C	18.46602583	-0.02004378	-0.32955719
I	17.33155253	-2.97429277	0.96585430
I	14.68046222	-3.25674834	-2.29655175
I	13.08631553	-5.44780854	0.90070588
I	7.69413553	6.36826674	1.43479622
I	5.52110717	5.20544265	-1.36278672
I	3.42782552	3.90409089	1.44106926
I	1.26245103	2.74370314	-1.36724744
I	19.24710312	-1.41339336	-1.76178009
C	8.54241201	-0.03874818	-0.10138272
O	16.15911074	0.20882046	3.28645226
O	15.77965716	-0.42456716	4.29087818
H	14.10843765	-1.45061879	3.60259853
O	13.34151557	-1.81889406	3.13305943
H	12.62144462	-1.77460206	3.78051984
H	14.71760480	-3.37312716	0.44221607

**b. Transition State 1**

C	2.20895633	1.17127779	-0.27866771
C	4.32671697	-0.04242227	-0.08324037
C	6.45645871	-1.27699637	-0.06722376
C	8.58404356	-2.51394409	-0.12788704
C	10.69970879	-3.76152365	-0.30937971
C	4.33910321	2.39795131	0.12392481
C	6.45529694	1.19049933	-0.08582255
C	10.00271465	-0.04832057	-0.08404362
C	10.70923495	-1.28629058	-0.13581828
C	12.80218770	-2.53355059	-0.26456902
C	6.46916870	3.63313293	-0.27548427
C	8.58690297	2.41865390	-0.08277381
C	10.71696647	1.18150100	-0.07441965
C	12.84996419	-0.05416908	-0.16553252
C	14.99111649	-1.29169539	-0.11663023

C	8.60174900	4.85906560	0.12505481
C	10.71885514	3.64961032	-0.08631506
C	12.85143237	2.41306748	-0.09040291
C	14.98178203	1.17118592	-0.09174940
C	17.11479831	-0.06749676	-0.22142470
C	3.60734537	1.20473908	-0.08161538
C	5.74514453	-0.03893130	-0.05694763
C	7.87607678	-1.27748564	-0.09072486
C	9.99797681	-2.51810581	-0.17309503
C	12.10424220	-3.72671681	-0.15660473
C	5.73742453	2.43807273	-0.08350873
C	7.87354567	1.19265592	-0.10485911
C	12.12015277	-1.28344808	-0.23392804
C	14.24137059	-2.55714710	-0.03428577
C	7.86836378	3.66641822	-0.07959875
C	10.00658612	2.42017541	-0.05929814
C	12.14157771	1.17757610	-0.09633802
C	14.27449222	-0.05676866	-0.16358587
C	16.37387069	-1.26349121	0.00043266
C	10.00069020	4.89681687	-0.08341987
C	12.13781616	3.64990780	-0.10694291
C	14.27032046	2.40942450	-0.07635230
C	16.40157098	1.17613045	-0.12012369
C	18.48335145	-0.02145991	-0.53837330
I	17.36927914	-2.89878363	0.95351391
I	15.13485215	-3.89267498	-1.72894879
I	13.03445509	-5.42351351	0.78818916
I	7.73209128	6.38518467	1.35169521
I	5.57750355	5.19021894	-1.44506859
I	3.46629754	3.91772620	1.35639229
I	1.32005513	2.72473776	-1.45409338
I	19.26779359	-1.46218163	-1.91836486
C	8.58325818	-0.04387014	-0.09000555

O	16.14531713	-0.17868400	2.62576674
O	15.60012116	-0.76825519	3.60171933
H	14.45154520	-1.76870972	3.07161586
O	13.81016969	-2.51846518	2.79611945
H	12.86512935	-2.36594656	2.95904242
H	14.08800583	-2.81168690	1.18775755

**c. Transition State 2**

C	2.20731007	1.17489977	-0.26500890
C	4.32786591	-0.04030621	-0.08237644
C	6.46268716	-1.27600839	-0.06819537
C	8.59783741	-2.51513247	-0.12596340
C	10.73238602	-3.76157987	-0.27462476
C	4.33930377	2.39966123	0.13464208
C	6.45891060	1.19197615	-0.08465177
C	10.01403463	-0.04908310	-0.07785199
C	10.73013913	-1.28959619	-0.10086673
C	12.86640647	-2.53016206	-0.28970771
C	6.46819011	3.63587555	-0.26218101
C	8.58897665	2.42085820	-0.08167753
C	10.72338561	1.18414243	-0.07215853
C	12.86033729	-0.05284462	-0.12954797
C	14.99563418	-1.29673743	-0.22912115
C	8.60080178	4.86146603	0.13696101
C	10.71970560	3.65246509	-0.08481631
C	12.85349096	2.41605952	-0.08892281
C	14.99101297	1.17290651	-0.06970725
C	17.12732659	-0.07038239	-0.22066306
C	3.60688629	1.20800013	-0.07458693
C	5.74782122	-0.03689379	-0.05892351
C	7.88428944	-1.27733613	-0.08957921
C	10.01671786	-2.51654240	-0.15739947
C	12.13775655	-3.73654515	-0.16505416
C	5.73759793	2.44057870	-0.07531708

C	7.87738499	1.19336503	-0.10642518
C	12.14947108	-1.28322320	-0.16443301
C	14.26458673	-2.46877565	-0.52521286
C	7.86772517	3.66975587	-0.07180571
C	10.00858132	2.42393242	-0.05996867
C	12.14504587	1.18416216	-0.09053751
C	14.27749865	-0.05301681	-0.12418944
C	16.39857917	-1.27227539	-0.07287796
C	9.99865417	4.90132500	-0.07519654
C	12.13814342	3.65398178	-0.10640005
C	14.27514441	2.41165020	-0.06905508
C	16.41026727	1.17687910	-0.12069678
C	18.50666377	-0.02025594	-0.50456731
I	17.32469316	-2.93669385	0.90003267
I	15.10141646	-3.84246150	-1.93765076
I	13.10598430	-5.40861959	0.77834534
I	7.72822446	6.38356424	1.36930482
I	5.56993629	5.19749922	-1.42407097
I	3.46465024	3.91465501	1.37405166
I	1.31205497	2.73326689	-1.43238329
I	19.28518826	-1.45435542	-1.89797434
C	8.59259798	-0.04529822	-0.09210509
O	16.18778561	-0.15779836	2.60078909
O	15.58175464	-0.87667552	3.57216922
H	14.93799843	-1.50142552	3.10357934
O	13.49420441	-2.45224022	2.84694037
H	12.58062559	-2.49944447	3.19085343
H	13.41145223	-2.63340427	1.89316040

**d. Transition State 3**

C	2.21890262	1.19397219	-0.25165599
C	4.34055425	-0.02108193	-0.07783824
C	6.47465588	-1.25880757	-0.06792263
C	8.60918110	-2.49658831	-0.15521837

C	10.74256227	-3.74197009	-0.31523756
C	4.35261600	2.41803281	0.14639675
C	6.47119586	1.20933266	-0.07872248
C	10.02589339	-0.02928952	-0.09172063
C	10.73922816	-1.26876936	-0.13741189
C	12.87687266	-2.50753429	-0.30823212
C	6.47984448	3.65448688	-0.24940240
C	8.60138835	2.43976866	-0.07721506
C	10.73620767	1.20394900	-0.07924939
C	12.87571235	-0.03241998	-0.16082075
C	15.01290567	-1.28783350	-0.23885241
C	8.61431753	4.87925707	0.14872118
C	10.73347569	3.67067732	-0.07917079
C	12.86739776	2.43403960	-0.09106027
C	15.00534880	1.18688932	-0.07898386
C	17.14205933	-0.05647814	-0.24724802
C	3.61929782	1.22771502	-0.06617534
C	5.76032160	-0.01903110	-0.05499392
C	7.89599002	-1.25944283	-0.09816495
C	10.02693298	-2.49694014	-0.20598564
C	12.14541579	-3.71069900	-0.18123299
C	5.75021416	2.45803476	-0.06392855
C	7.88973617	1.21238850	-0.10216310
C	12.16005494	-1.26120207	-0.20173199
C	14.27578282	-2.45711273	-0.52501970
C	7.87997545	3.68904056	-0.06307958
C	10.02125168	2.44290224	-0.05799881
C	12.15884446	1.20270405	-0.10375087
C	14.29360757	-0.03987727	-0.13866349
C	16.41698500	-1.26166142	-0.09705280
C	10.01186144	4.91908695	-0.06338345
C	12.15203845	3.67252072	-0.10218347
C	14.28928313	2.42742972	-0.07244727



C	16.42447605	1.19258970	-0.13653775
C	18.52062175	-0.00413896	-0.53600354
I	17.36951902	-2.94042007	0.85110383
I	15.10873764	-3.83382969	-1.94198998
I	13.09247204	-5.34606677	0.82791176
I	7.74125502	6.40005838	1.38105802
I	5.58364048	5.21326440	-1.41684644
I	3.47896069	3.93429369	1.38330446
I	1.32285637	2.75228452	-1.41947075
I	19.30472853	-1.43683521	-1.92496747
C	8.60412608	-0.02679721	-0.09602644
O	16.24266577	-0.28357761	2.42055309
O	15.37980759	-0.82564783	3.30501333
H	15.31152572	-1.78530473	3.05818302
O	12.91234607	-2.22018099	3.19303040
H	12.07478134	-2.62922534	3.45694165
H	12.82721777	-2.14262239	2.22626571

**e. Transition State 4**

C	2.21859396	1.20523784	-0.24409036
C	4.34051910	-0.00795880	-0.07322603
C	6.47416076	-1.24541886	-0.07155906
C	8.60767927	-2.48093117	-0.19351113
C	10.74044526	-3.72462794	-0.38170716
C	4.35354673	2.42891024	0.15399373
C	6.47096008	1.22130428	-0.07391400
C	10.02394589	-0.01252985	-0.11297095
C	10.73689515	-1.24871290	-0.18933583
C	12.88077192	-2.48648331	-0.36272575
C	6.48014871	3.66524857	-0.24338737
C	8.60132309	2.45364698	-0.07272330
C	10.73629044	1.21898267	-0.08907620
C	12.87553484	-0.01736342	-0.18710043
C	15.01870920	-1.27218611	-0.23371820

C	8.61555423	4.89050326	0.15906945
C	10.73350785	3.68256792	-0.07452803
C	12.86830718	2.44727053	-0.09189711
C	15.00646558	1.20014786	-0.07927985
C	17.14250785	-0.04328896	-0.24327101
C	3.61906275	1.24053132	-0.05862177
C	5.75996705	-0.00707163	-0.05317696
C	7.89486737	-1.24492721	-0.11529726
C	10.02473531	-2.47692725	-0.25698067
C	12.14869355	-3.69566052	-0.26154650
C	5.75041590	2.46930128	-0.05625002
C	7.88895661	1.22576617	-0.09995246
C	12.15876048	-1.24256468	-0.24812730
C	14.28408406	-2.43764462	-0.55560761
C	7.88019824	3.70164397	-0.05477349
C	10.02116115	2.45554224	-0.05696097
C	12.15909410	1.21680549	-0.11692432
C	14.29646718	-0.02755535	-0.14421452
C	16.41788669	-1.24416815	-0.04314169
C	10.01224405	4.93078664	-0.05374254
C	12.15274828	3.68501860	-0.09931806
C	14.29069521	2.43946097	-0.07321444
C	16.42543829	1.20651378	-0.15144292
C	18.51495791	0.00932121	-0.57266237
I	17.39542488	-2.96006614	0.81990009
I	15.14327958	-3.79879565	-1.96714129
I	13.09189136	-5.33532465	0.73928453
I	7.74008151	6.41083700	1.38859040
I	5.58496992	5.21849922	-1.41764676
I	3.47882906	3.94604785	1.38968168
I	1.32526311	2.75696544	-1.42267167
I	19.26249787	-1.42909573	-1.97805729
C	8.60263798	-0.01169762	-0.10527254

O	16.22304821	-0.35224701	2.32757708
O	15.16069253	-1.07672754	2.75934238
H	15.53147486	-1.94725690	3.05785586
O	12.77861118	-2.13362989	3.25456264
H	11.95522706	-2.60297386	3.45763770
H	12.79609848	-2.07451284	2.28944763

**f. Transition State 5**

C	2.21775680	1.21151821	-0.24010857
C	4.33883689	0.00075212	-0.06914635
C	6.47282950	-1.23624336	-0.07472623
C	8.60669975	-2.46998214	-0.21582849
C	10.73311338	-3.70504367	-0.43652515
C	4.35276784	2.43548702	0.16229803
C	6.46993736	1.22935879	-0.07005375
C	10.02373523	-0.00555016	-0.12577388
C	10.73489364	-1.23722713	-0.21066677
C	12.88096885	-2.46842766	-0.41182785
C	6.47918112	3.67123008	-0.24038423
C	8.59989982	2.46147382	-0.06985570
C	10.73554630	1.22806459	-0.09498453
C	12.87354356	-0.00798175	-0.19553589
C	15.01595200	-1.26163688	-0.22631495
C	8.61533078	4.89508527	0.16557150
C	10.73260042	3.68996879	-0.07183586
C	12.86694625	2.45612001	-0.09130362
C	15.00595559	1.20945941	-0.06869838
C	17.14696749	-0.02254426	-0.25551595
C	3.61911993	1.24604612	-0.05274951
C	5.75975992	-0.00147522	-0.05146825
C	7.89450880	-1.23645836	-0.12783463
C	10.02254901	-2.46688931	-0.28306851
C	12.14813309	-3.68376784	-0.32812679
C	5.75039095	2.47503013	-0.04963231

C	7.88852656	1.23248764	-0.09955439
C	12.15903638	-1.23253447	-0.26711754
C	14.28623733	-2.41150963	-0.58498782
C	7.88017440	3.70678648	-0.05060178
C	10.02143968	2.46164175	-0.05596400
C	12.15829494	1.22416412	-0.12206668
C	14.29590150	-0.02303833	-0.13898864
C	16.41467000	-1.20658830	0.08789031
C	10.01209855	4.93542417	-0.04829300
C	12.15311438	3.69088000	-0.09875675
C	14.29182008	2.44422128	-0.07077546
C	16.42842600	1.21385912	-0.15743119
C	18.50416066	0.03044957	-0.62339291
I	17.41726288	-2.98851343	0.80793706
I	15.16790203	-3.78640341	-1.97219590
I	13.07789675	-5.30952815	0.71471377
I	7.73905679	6.41536576	1.39234717
I	5.58584201	5.22102369	-1.41932445
I	3.47721908	3.95194841	1.39433808
I	1.32765730	2.75617810	-1.42662098
I	19.24579340	-1.44406565	-1.98452369
C	8.60056328	-0.00290226	-0.11175338
O	16.21598269	-0.56381950	2.05102255
O	15.10662766	-1.29424928	2.49160812
H	15.51063506	-1.99118972	3.06445698
O	12.78047508	-2.14162460	3.30928410
H	11.92730884	-2.55849315	3.49987968
H	12.80732172	-2.07942428	2.34488463

**g. Final**

C	2.21548016	1.22015458	-0.24043970
C	4.33595193	0.00945488	-0.06836401
C	6.47007775	-1.22719229	-0.07986770
C	8.60095623	-2.46144765	-0.18972874

C	10.73338615	-3.70459565	-0.42353038
C	4.35093259	2.44389095	0.16412773
C	6.46655815	1.23785598	-0.07159646
C	10.01803074	0.00475931	-0.12470482
C	10.73053998	-1.23291696	-0.22296383
C	12.86883244	-2.46180093	-0.43826373
C	6.47584207	3.68129021	-0.23788699
C	8.59570936	2.47158977	-0.06921550
C	10.72745562	1.23626640	-0.09933409
C	12.86078995	0.00257854	-0.19485087
C	14.97458657	-1.26314592	-0.13446191
C	8.61284647	4.90533735	0.16534768
C	10.72920957	3.69889739	-0.07274941
C	12.86067467	2.46415950	-0.09742753
C	14.99486714	1.22099137	-0.01764257
C	17.15900572	-0.00631515	-0.11157883
C	3.61561538	1.25684918	-0.05022450
C	5.75573510	0.00953489	-0.05538593
C	7.88846840	-1.22526823	-0.12881743
C	10.02116581	-2.46242246	-0.28633381
C	12.14667743	-3.67557791	-0.34114080
C	5.74658636	2.48517966	-0.04807572
C	7.88506942	1.24318074	-0.10057276
C	12.14930123	-1.22715004	-0.28924718
C	14.30068765	-2.38912940	-0.56783953
C	7.87516159	3.71948887	-0.04730393
C	10.01504918	2.47236837	-0.06020665
C	12.14891949	1.23698659	-0.13117147
C	14.26946674	-0.01121304	-0.07825277
C	16.36111329	-1.15876066	0.45697212
C	10.00889716	4.94576195	-0.04884913
C	12.14794729	3.70159694	-0.09898195
C	14.28533043	2.45533218	-0.07133869

C	16.42678390	1.23304154	-0.06785544
C	18.48248562	0.00668508	-0.52170218
I	17.43349290	-3.11576324	0.92117492
I	15.25046843	-3.73128547	-1.94384568
I	13.12863290	-5.32489070	0.62598362
I	7.73641760	6.43064647	1.38749007
I	5.58125527	5.23185776	-1.41542759
I	3.46966106	3.96603525	1.38669756
I	1.32199246	2.76797171	-1.42225001
I	19.17852123	-1.51650541	-1.86112144
C	8.59814535	0.00653555	-0.11385540
O	16.20611937	-0.66712537	1.82033687
O	15.07818514	-1.32210039	2.48571249
H	15.52528662	-2.09383728	2.90155168
O	12.69901849	-2.19410951	3.39751791
H	11.75492492	-2.28261131	3.59186445
H	12.75278950	-2.03557807	2.43866088

**2) O formation**  
**a. Initial**

C	2.22036726	1.22410892	-0.25111045
C	4.33992101	0.01825705	-0.06847098
C	6.47421142	-1.21217669	-0.08317795
C	8.60562107	-2.44187466	-0.20425360
C	10.72735105	-3.69283738	-0.41559068
C	4.35445616	2.44930981	0.16673932
C	6.46965406	1.24943734	-0.07203537
C	10.02298832	0.01570673	-0.14693628
C	10.73590845	-1.21935772	-0.23492366
C	12.86031198	-2.46976216	-0.27756748
C	6.48005150	3.68917442	-0.24730287
C	8.60014619	2.48126883	-0.07230078
C	10.73308677	1.24370121	-0.11178064
C	12.86460526	0.00573936	-0.22106914

C	14.97180838	-1.22083240	-0.02853864
C	8.61800729	4.90987754	0.16862065
C	10.73292360	3.70554803	-0.07517294
C	12.86553905	2.47336556	-0.10593369
C	15.00176639	1.24640144	-0.04785090
C	17.14619951	0.01623461	-0.14435118
C	3.61906780	1.26376050	-0.05202899
C	5.75951498	0.02036882	-0.05419285
C	7.89319610	-1.21139548	-0.13988489
C	10.02544796	-2.44820894	-0.28168438
C	12.13851670	-3.67097023	-0.25515477
C	5.74918351	2.49542057	-0.05065545
C	7.88951392	1.25319520	-0.10426632
C	12.15386295	-1.22635822	-0.28186574
C	14.32017381	-2.45961594	-0.24790898
C	7.87866642	3.72809981	-0.05066880
C	10.02018634	2.47817881	-0.06299768
C	12.15720479	1.23726073	-0.14983272
C	14.29108202	0.00139341	-0.11457188
C	16.36892995	-1.11124708	0.48544530
C	10.01316872	4.95095326	-0.05093807
C	12.15434141	3.70634918	-0.10333758
C	14.29150499	2.47141950	-0.08060001
C	16.42671737	1.25466750	-0.08959329
C	18.46376314	0.03674296	-0.58708289
I	17.46210289	-3.11038064	0.73938532
I	15.14258570	-3.34118012	-2.43316920
I	13.15479368	-5.43795609	0.39227279
I	7.74709681	6.43460483	1.38866074
I	5.58694518	5.23731317	-1.42091184
I	3.47104349	3.96813379	1.38511370
I	1.33055118	2.76227225	-1.43875216
I	19.08851857	-1.40241295	-2.03640124

C	8.60283254	0.02016661	-0.12485272
O	16.36237543	-0.60600488	1.84681964
O	15.47993366	-1.44154415	2.68021417
H	16.02142636	-2.26752546	2.74055252
H	13.62059261	-1.56407130	3.23848059
O	12.82547922	-2.12132712	3.30396928
H	12.41557821	-1.87458699	4.14539251
H	14.76824274	-3.31265163	0.26080946

**b. Transition State 1**

C	2.22023705	1.22407220	-0.24634841
C	4.34061299	0.01942341	-0.06440741
C	6.47435048	-1.20816214	-0.08770504
C	8.60333749	-2.43802308	-0.20894400
C	10.72163452	-3.68616951	-0.41925879
C	4.35206463	2.45404150	0.16274275
C	6.46913072	1.25181385	-0.06751535
C	10.02172411	0.01938174	-0.14270985
C	10.73394669	-1.21569830	-0.23376953
C	12.84349444	-2.46930633	-0.30300991
C	6.47905415	3.69222442	-0.24281014
C	8.59955568	2.48427611	-0.06605021
C	10.73172238	1.24607488	-0.11275054
C	12.86093361	0.00762645	-0.27009568
C	14.96985445	-1.21337350	-0.08883686
C	8.61600510	4.91430684	0.16964466
C	10.73339963	3.70604012	-0.06848408
C	12.86542792	2.47375375	-0.12223086
C	15.00288721	1.25081405	-0.11238073
C	17.15422504	0.01895929	-0.14553267
C	3.61966145	1.26459551	-0.04787643
C	5.75938613	0.02352923	-0.05119795
C	7.89159791	-1.20779411	-0.14125137
C	10.02505860	-2.44368497	-0.28230370



C	12.12943571	-3.67156181	-0.25024853
C	5.74873368	2.49650180	-0.04791978
C	7.88883010	1.25683023	-0.09964503
C	12.14716183	-1.22699734	-0.30463514
C	14.30271709	-2.46162610	-0.29419501
C	7.87830807	3.73014105	-0.04527385
C	10.01922088	2.48008796	-0.05853592
C	12.15438646	1.24061008	-0.17333323
C	14.28427142	0.01270678	-0.21693903
C	16.33872501	-1.08578036	0.50583192
C	10.01315751	4.95100368	-0.04321234
C	12.15384035	3.70838374	-0.10121539
C	14.29222391	2.47553581	-0.10961984
C	16.43156666	1.25922709	-0.10255707
C	18.45702154	0.04341072	-0.59623749
I	17.49701201	-3.20901570	0.73115558
I	15.12371420	-3.38006042	-2.38445567
I	13.13522315	-5.42387875	0.43225898
I	7.74028177	6.44403754	1.38064448
I	5.59014729	5.23630266	-1.42999836
I	3.46595704	3.97782961	1.37124171
I	1.32945362	2.75855044	-1.44409253
I	19.09146798	-1.41578755	-2.02031142
C	8.60223171	0.02398931	-0.12035648
O	16.12408775	-0.68384193	1.74342063
O	15.62473490	-1.90262703	3.61691871
H	16.18769113	-2.44263666	3.00572258
H	13.98122453	-2.08001434	3.14612044
O	13.05570596	-2.18161444	2.79408984
H	12.49494938	-2.19504753	3.58724950
H	14.75314098	-3.27347201	0.28312997

**c. Transition State 2**

C	2.21627370	1.22943791	-0.24566249
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C	4.33656079	0.02247283	-0.06411017
C	6.47355613	-1.20530381	-0.08739556
C	8.60562901	-2.44395373	-0.19432531
C	10.72484248	-3.68258675	-0.42314590
C	4.34948736	2.45746492	0.15981191
C	6.46715410	1.25403359	-0.06733926
C	10.02071015	0.02342269	-0.14086196
C	10.73607359	-1.21128079	-0.23130171
C	12.83392843	-2.46190662	-0.31359129
C	6.47670976	3.69468509	-0.24213816
C	8.59826753	2.48470511	-0.06649359
C	10.73166484	1.24909570	-0.11418683
C	12.87185705	0.01848813	-0.27573678
C	14.98198426	-1.21024772	-0.03003806
C	8.61349820	4.91659681	0.16504169
C	10.73157196	3.71033844	-0.07000408
C	12.86563694	2.47791812	-0.12556121
C	14.99913081	1.25192916	-0.12080083
C	17.17150917	0.01412299	-0.15502410
C	3.61505772	1.26899985	-0.04941383
C	5.75692287	0.02709562	-0.05161770
C	7.89077880	-1.20786292	-0.13662763
C	10.02518527	-2.44213117	-0.27640283
C	12.13181861	-3.66425317	-0.26133313
C	5.74576418	2.50018448	-0.04930793
C	7.88649435	1.25758791	-0.09893647
C	12.14600520	-1.22027575	-0.30756185
C	14.28526037	-2.46363625	-0.34048105
C	7.87602247	3.73175474	-0.04673126
C	10.01764526	2.48340524	-0.06007288
C	12.15537358	1.24804125	-0.17776576
C	14.28129112	0.04403440	-0.23326111
C	16.41998993	-1.17696620	0.32364019

C	10.01034798	4.95583929	-0.04713548
C	12.15000369	3.71482817	-0.10112019
C	14.28758970	2.48362699	-0.11311325
C	16.43709546	1.24868677	-0.09643146
C	18.47720555	0.04981741	-0.60428809
I	17.52142619	-3.14609663	0.70813717
I	15.10484269	-3.41894073	-2.33574215
I	13.13238815	-5.41621515	0.43949118
I	7.73856933	6.44551696	1.38078061
I	5.58831221	5.23893401	-1.42955043
I	3.46342419	3.98304276	1.37218628
I	1.32637616	2.76406375	-1.44409312
I	19.11182898	-1.40438893	-2.04066391
C	8.60094061	0.02282830	-0.11916044
O	15.69311083	-0.96100624	1.46818598
O	15.63787165	-1.87914938	3.77181586
H	16.14194189	-2.37741239	3.08907035
H	14.03029516	-2.07660413	3.22123339
O	13.15395164	-2.25278128	2.77803336
H	12.51224700	-2.24934033	3.50144634
H	14.70071439	-3.26063991	0.28666589

**d. Transition State 3**

C	2.20396657	1.23901158	-0.25074774
C	4.32279393	0.02831103	-0.06551826
C	6.45820726	-1.20242247	-0.08639883
C	8.58962584	-2.44407039	-0.18652912
C	10.70671534	-3.67626990	-0.44051987
C	4.33834069	2.46495114	0.15227276
C	6.45468018	1.25861105	-0.06647413
C	10.00573174	0.02805504	-0.17370371
C	10.71877645	-1.20570115	-0.28255781
C	12.81282715	-2.45881499	-0.40277646
C	6.46624291	3.69950848	-0.24763718

C	8.58533575	2.48790947	-0.06791510
C	10.71691786	1.25561070	-0.15230763
C	12.85259964	0.02830647	-0.37813857
C	14.95309116	-1.20797518	-0.06596264
C	8.60156852	4.92303766	0.15714672
C	10.71678143	3.71825747	-0.08020110
C	12.84821225	2.48356436	-0.15595179
C	14.97820612	1.25464565	-0.16065290
C	17.15142440	0.01750005	-0.20588479
C	3.60220439	1.27676980	-0.05378470
C	5.74373559	0.03150859	-0.05005629
C	7.87630126	-1.20724234	-0.12746382
C	10.00694090	-2.43856794	-0.28477282
C	12.11518142	-3.65843746	-0.30835204
C	5.73458368	2.50593280	-0.05499320
C	7.87348334	1.25968314	-0.09766548
C	12.12602820	-1.21357686	-0.41633134
C	14.26780365	-2.46564641	-0.38676708
C	7.86465350	3.73611329	-0.04994047
C	10.00473120	2.48939424	-0.07157634
C	12.13713564	1.25621861	-0.24086176
C	14.25719690	0.05765613	-0.31319432
C	16.42441750	-1.20626221	0.19254259
C	9.99694336	4.96502672	-0.05712313
C	12.13485307	3.72132830	-0.10977405
C	14.26916807	2.48957496	-0.13483292
C	16.41786816	1.24679891	-0.11284875
C	18.46594980	0.06147077	-0.63858683
I	17.57836595	-3.06485429	0.63037804
I	15.08597119	-3.45782103	-2.28702863
I	13.10089912	-5.40179843	0.43589876
I	7.72248210	6.44987149	1.37313867
I	5.57970313	5.24125637	-1.43904357

I	3.45506652	3.99275291	1.36423170
I	1.31230972	2.77702349	-1.44294048
I	19.12712241	-1.32105377	-2.13869528
C	8.58653968	0.02371580	-0.12021072
O	15.56349253	-1.06131933	1.28977605
O	15.32959424	-1.76408735	4.08019895
H	16.07853922	-1.95580124	3.48760685
H	14.53493637	-1.90002513	3.45760404
O	13.50214809	-2.42285785	2.42971872
H	12.70880305	-2.86023996	2.78346567
H	14.63426586	-3.22532484	0.30530381

**e. Transition State 4**

C	2.20816652	1.24399422	-0.25083925
C	4.32759344	0.03366900	-0.06393458
C	6.46306444	-1.19810386	-0.08484560
C	8.59254756	-2.43874084	-0.18660068
C	10.70485110	-3.67206576	-0.45525827
C	4.34151987	2.47060959	0.14976412
C	6.45903941	1.26423314	-0.06592640
C	10.00916647	0.03417731	-0.18623530
C	10.71992529	-1.20075501	-0.29061059
C	12.80431701	-2.46124515	-0.45603562
C	6.47042600	3.70549398	-0.24909015
C	8.59005340	2.49379000	-0.06990989
C	10.72083139	1.26143181	-0.16931386
C	12.85581561	0.03040883	-0.38836076
C	14.95602654	-1.21840485	-0.07986438
C	8.60609338	4.92734889	0.15817142
C	10.72288839	3.72352382	-0.08035681
C	12.85545813	2.48767948	-0.17336958
C	14.98141852	1.25585471	-0.16280336
C	17.15150434	0.02385137	-0.22226820
C	3.60598165	1.28185797	-0.05368517

C	5.74828749	0.03634761	-0.04848120
C	7.88065408	-1.20126209	-0.12597930
C	10.00842483	-2.43355113	-0.28927074
C	12.11217373	-3.66526157	-0.35530874
C	5.73815260	2.51222186	-0.05646818
C	7.87804492	1.26575270	-0.09935830
C	12.12553866	-1.21084625	-0.42802621
C	14.25034693	-2.46765657	-0.43305311
C	7.86851402	3.74159576	-0.05095567
C	10.00951748	2.49485009	-0.07693476
C	12.14164063	1.26153592	-0.25753709
C	14.26004471	0.05547871	-0.31299785
C	16.42707601	-1.20015891	0.17585005
C	10.00195891	4.97017867	-0.05560789
C	12.14123883	3.72593935	-0.11309013
C	14.27490198	2.49218139	-0.13871728
C	16.42016295	1.25185026	-0.11574275
C	18.46231259	0.06908453	-0.65435265
I	17.58167939	-3.05962015	0.60501600
I	15.06709969	-3.49670133	-2.23831510
I	13.07730504	-5.44972277	0.34958192
I	7.72854875	6.45332442	1.37655206
I	5.58530679	5.24972067	-1.43946962
I	3.45819345	3.99991706	1.36096765
I	1.31529405	2.78126914	-1.44411374
I	19.09944968	-1.30162834	-2.17831797
C	8.59103573	0.03002906	-0.12423594
O	15.58812316	-1.04655655	1.27911007
O	15.23995204	-1.77938970	4.10233735
H	16.04081931	-1.98779936	3.59628500
H	14.55712604	-1.94947982	3.40553590
O	13.94961993	-2.80029656	2.06676313
H	13.00614401	-2.93108706	2.30893087

H	14.37883231	-3.13854992	0.78779319
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**f. Transition State 5**

C	2.19730454	1.22885646	-0.25088019
C	4.31256525	0.01423101	-0.07669951
C	6.44521416	-1.21894581	-0.09532123
C	8.57538231	-2.45840038	-0.18328896
C	10.68799596	-3.69597077	-0.45412624
C	4.33291757	2.45315495	0.15759087
C	6.44445500	1.24518250	-0.06929955
C	9.99479584	0.01177292	-0.14831009
C	10.71022910	-1.22572443	-0.23777614
C	12.81005812	-2.48782394	-0.41176898
C	6.45875353	3.68800625	-0.24554233
C	8.57552568	2.47626186	-0.06754271
C	10.70473170	1.24075435	-0.13752096
C	12.83644624	0.00874680	-0.33623065
C	14.93840108	-1.25137633	-0.09005829
C	8.59488481	4.91358816	0.15813362
C	10.70597944	3.70667407	-0.08942266
C	12.83367260	2.46758835	-0.18759488
C	14.96489129	1.23071636	-0.16711622
C	17.13675907	-0.00171575	-0.20142610
C	3.59548090	1.26502956	-0.05296214
C	5.73301489	0.01703737	-0.05970939
C	7.86235901	-1.22063281	-0.12436198
C	9.99193522	-2.45620061	-0.27562010
C	12.09465882	-3.68875247	-0.35825584
C	5.72700126	2.49376995	-0.05326208
C	7.86297239	1.24716701	-0.09738297
C	12.11723694	-1.22991782	-0.34046734
C	14.23289021	-2.46966672	-0.47933914
C	7.85700648	3.72587469	-0.04826262
C	9.99427919	2.47788308	-0.07282477

C	12.12263783	1.24044491	-0.23427737
C	14.24004225	0.03009839	-0.30040254
C	16.40085472	-1.22707894	0.19558443
C	9.98863434	4.95479398	-0.05979842
C	12.12263055	3.70744582	-0.13074886
C	14.25572304	2.46995683	-0.15421272
C	16.40467961	1.23022999	-0.11638723
C	18.44887433	0.03974494	-0.63891854
I	17.55001013	-3.08423329	0.64098073
I	15.04822819	-3.53558163	-2.18960158
I	13.09594654	-5.40728688	0.45175764
I	7.71626773	6.44879931	1.36573736
I	5.57599801	5.23206639	-1.44253744
I	3.45105715	3.99156019	1.35879623
I	1.30913156	2.77230637	-1.44261386
I	19.12500480	-1.35102912	-2.12741138
C	8.57392959	0.00901059	-0.11285408
O	15.54017157	-1.09234990	1.29735769
O	15.46390530	-1.68513112	4.10381135
H	16.16263741	-1.88186897	3.46435458
H	14.64770962	-1.85286050	3.59320590
O	13.22306691	-2.28815318	2.44488970
H	12.80069015	-3.10366600	2.74455772
H	13.79897098	-2.59986795	1.71425589

**g. Final**

C	2.16766151	1.19735349	-0.20525888
C	4.28823644	-0.01623868	-0.07001450
C	6.42469128	-1.24615019	-0.08980069
C	8.56222116	-2.48805355	-0.11355274
C	10.69075081	-3.72833974	-0.28753479
C	4.30386923	2.41645115	0.20407444
C	6.41797220	1.21744812	-0.06615029
C	9.97526865	-0.02016874	-0.09818787



C	10.69626184	-1.25872332	-0.12635989
C	12.81931073	-2.51431510	-0.30217440
C	6.42804663	3.65805627	-0.20254194
C	8.54929898	2.44581482	-0.06245540
C	10.67968810	1.21253018	-0.10982295
C	12.81376605	-0.01384214	-0.28784511
C	14.91530469	-1.27576778	-0.10747940
C	8.56597464	4.87732838	0.20308692
C	10.67973176	3.67746290	-0.07800646
C	12.81366032	2.44251380	-0.16817372
C	14.94757739	1.20610343	-0.15388294
C	17.12009968	-0.02892201	-0.09749727
C	3.56749300	1.23130110	-0.02261955
C	5.70934602	-0.01134054	-0.05974924
C	7.84380503	-1.24954184	-0.09863381
C	9.98013548	-2.49012373	-0.15216495
C	12.09687880	-3.71594635	-0.18259572
C	5.69569551	2.46539424	-0.02465183
C	7.83680477	1.21831986	-0.09809192
C	12.10419087	-1.25768696	-0.23748668
C	14.21543349	-2.47167688	-0.52562517
C	7.82821759	3.69318367	-0.02079946
C	9.96737308	2.44936474	-0.06513571
C	12.09803440	1.21753891	-0.20104163
C	14.22142472	0.00880565	-0.29034955
C	16.35647480	-1.25362556	0.26179133
C	9.95811886	4.92499284	-0.02818956
C	12.09788930	3.67961097	-0.12249461
C	14.23550667	2.44314840	-0.14207380
C	16.38450435	1.20222042	-0.07078278
C	18.45460626	0.00398355	-0.47488451
I	17.47829722	-3.12808164	0.73853463
I	15.02935668	-3.57446193	-2.14088805

I	13.12449631	-5.38143699	0.66696833
I	7.70344334	6.37527420	1.46269284
I	5.52389401	5.22861951	-1.34175125
I	3.43948961	3.91274158	1.46437907
I	1.26440358	2.76863845	-1.34363134
I	19.17421630	-1.40006025	-1.93265893
C	8.55253914	-0.01910578	-0.09724390
O	15.45313936	-1.13746572	1.32274121
O	15.86806675	-1.44098808	4.09884773
H	16.23965482	-1.86322399	3.30675551
H	14.90671803	-1.54012285	3.96039751
O	13.14841062	-1.94362931	3.20711475
H	12.21959002	-1.81382684	3.44606561
H	13.18377435	-1.81483103	2.24376058

### 3) OH formation

#### a. Initial

C	2.16456651	1.19361047	-0.20168421
C	4.28449865	-0.01973591	-0.06195527
C	6.41860919	-1.24989061	-0.08444900
C	8.55061186	-2.48560356	-0.16104625
C	10.67595121	-3.71292475	-0.43419254
C	4.29877477	2.41371682	0.20710125
C	6.41265633	1.21499163	-0.06208679
C	9.96842108	-0.01958531	-0.12936156
C	10.68544762	-1.25583801	-0.20415352
C	12.78505618	-2.51849739	-0.31366162
C	6.42453554	3.65558270	-0.19502848
C	8.54613739	2.44319852	-0.06139087
C	10.67701179	1.20920334	-0.11428503
C	12.81692426	-0.02651310	-0.26284230
C	14.93328287	-1.27683618	-0.04554864
C	8.56278901	4.87443837	0.20443795
C	10.67750646	3.67361266	-0.07240188

C	12.81250394	2.43526352	-0.13740848
C	14.94715230	1.19518296	-0.11313848
C	17.12635564	-0.02783955	-0.22878147
C	3.56446864	1.22670351	-0.01819153
C	5.70453204	-0.01449835	-0.05434549
C	7.83610843	-1.24941522	-0.11354056
C	9.97053494	-2.48238334	-0.24995860
C	12.08500662	-3.71369573	-0.32201567
C	5.69162055	2.46192410	-0.01846583
C	7.83198413	1.21716811	-0.09779587
C	12.09479772	-1.27042212	-0.27943164
C	14.24507171	-2.52168522	-0.45072306
C	7.82574591	3.68924955	-0.01643833
C	9.96497102	2.44526206	-0.06453270
C	12.09926645	1.20842654	-0.17937953
C	14.22265695	-0.00405625	-0.23125364
C	16.40570942	-1.27809041	0.11794206
C	9.95611531	4.92040207	-0.02508190
C	12.09596786	3.67483081	-0.10928525
C	14.23527872	2.43467630	-0.11256905
C	16.38766777	1.19816312	-0.09460632
C	18.43522138	0.03683656	-0.68311832
I	17.51561779	-3.19839722	0.22302251
I	14.67526841	-2.65970775	-2.68999949
I	13.12822992	-5.52498793	0.14281746
I	7.69956662	6.37807909	1.46260889
I	5.51903485	5.22807026	-1.33584181
I	3.42933662	3.91435460	1.46404078
I	1.25977485	2.76568479	-1.34306375
I	19.03123235	-1.18663118	-2.34795441
C	8.54707624	-0.01872899	-0.11165611
O	15.61113258	-1.22168024	1.29614769
H	14.30985581	-2.09163110	2.55660849

O	13.43734378	-2.51340855	2.62822092
H	12.94863821	-1.96023331	3.25656520
H	14.73521940	-3.42051766	-0.06987998

**b. Transition State 1**

C	2.17268068	1.19587760	-0.21890260
C	4.29068615	-0.01288766	-0.05966069
C	6.42221645	-1.23963595	-0.08971560
C	8.55060770	-2.46425709	-0.20211273
C	10.67198684	-3.71670074	-0.41598544
C	4.30421120	2.42105411	0.19738699
C	6.41637901	1.22385116	-0.06581263
C	9.96882012	-0.01272974	-0.15395498
C	10.68077403	-1.24796781	-0.23609062
C	12.78773598	-2.50509607	-0.25989196
C	6.42988692	3.66258806	-0.20920102
C	8.54944480	2.45211877	-0.06472291
C	10.67874100	1.21480125	-0.11709119
C	12.81083905	-0.02356047	-0.23416199
C	14.92655665	-1.24154794	-0.04934406
C	8.57001357	4.88229115	0.19506413
C	10.68185240	3.67744105	-0.07121783
C	12.81488376	2.44189192	-0.11908305
C	14.95803235	1.21518799	-0.07263112
C	17.11356309	-0.00790087	-0.12053450
C	3.57199804	1.23173504	-0.02335465
C	5.70939584	-0.00656600	-0.05428112
C	7.83759033	-1.23502352	-0.14433588
C	9.97123394	-2.47426651	-0.28426504
C	12.07895330	-3.70728237	-0.23821577
C	5.69681546	2.46913815	-0.02584464
C	7.83544532	1.22661236	-0.10500376
C	12.09599176	-1.25856555	-0.27797156
C	14.25184073	-2.49826753	-0.23815290

C	7.83079813	3.69779378	-0.02338705
C	9.96880497	2.45038194	-0.06449745
C	12.10131318	1.21006851	-0.16140157
C	14.23504212	-0.02325417	-0.14390217
C	16.29916686	-1.10778612	0.55920050
C	9.96316748	4.92331667	-0.03140113
C	12.10268208	3.67680281	-0.10466374
C	14.24337643	2.44041372	-0.09814393
C	16.38698942	1.22980354	-0.08182243
C	18.40812975	0.01471704	-0.59032332
I	17.48273751	-3.35234519	0.64358182
I	14.98734310	-2.98010071	-2.40480956
I	13.09635392	-5.46365762	0.41561707
I	7.70590201	6.40065129	1.43103097
I	5.53053402	5.22433031	-1.36586919
I	3.42385953	3.92929668	1.43379915
I	1.27889178	2.74922114	-1.38849006
I	19.04201235	-1.45401571	-2.00311383
C	8.54815348	-0.00614828	-0.13319142
O	16.18523952	-0.84745342	1.81588700
H	14.79737952	-1.76075726	2.55513355
O	13.95104253	-2.26280732	2.62229925
H	13.33913317	-1.67760121	3.08541114
H	14.72446811	-3.32755923	0.29456088

**c. Transition State 2**

C	2.17196430	1.19784869	-0.22140731
C	4.28881832	-0.01052720	-0.05834993
C	6.41850552	-1.23727409	-0.09426313
C	8.54410466	-2.46028735	-0.21746803
C	10.66150967	-3.71508633	-0.40877138
C	4.30321472	2.42384229	0.19884256
C	6.41433795	1.22690161	-0.06468872
C	9.96557446	-0.01035359	-0.16461231

C	10.67543302	-1.24623507	-0.24832498
C	12.77529586	-2.51388743	-0.21143192
C	6.42918761	3.66524562	-0.21211836
C	8.54814929	2.45476434	-0.06453302
C	10.67714511	1.21583029	-0.12226683
C	12.81003369	-0.02735227	-0.24482224
C	14.92522473	-1.24326208	-0.01538819
C	8.56933254	4.88464288	0.19711147
C	10.68043492	3.67964430	-0.07045638
C	12.81228201	2.44230376	-0.12722744
C	14.95455015	1.21670597	-0.09594943
C	17.10791641	-0.00409869	-0.11629812
C	3.57090605	1.23451928	-0.02279985
C	5.70708251	-0.00378437	-0.05332082
C	7.83260893	-1.23140337	-0.15524098
C	9.96414643	-2.47063391	-0.29630851
C	12.05869736	-3.71148328	-0.17352449
C	5.69558910	2.47224932	-0.02624940
C	7.83340820	1.22955672	-0.10578672
C	12.09147886	-1.26289903	-0.27903457
C	14.24056445	-2.51590547	-0.08535589
C	7.82997495	3.70080169	-0.02390237
C	9.96771176	2.45216536	-0.06499650
C	12.10006059	1.20895137	-0.17227186
C	14.23596426	-0.02676290	-0.16653068
C	16.29734909	-1.08856120	0.59314024
C	9.96229664	4.92568999	-0.03093857
C	12.10110928	3.67829690	-0.10524892
C	14.24013543	2.44215072	-0.11189947
C	16.38219601	1.23431760	-0.09421455
C	18.40261055	0.01322779	-0.58160641
I	17.52725429	-3.21062497	0.89392559
I	15.10997473	-3.35875937	-2.05953273

I	13.00308413	-5.44674216	0.62209268
I	7.70646048	6.40041511	1.43569175
I	5.53126405	5.22673461	-1.36926961
I	3.42386952	3.93165855	1.43542836
I	1.27815789	2.74986002	-1.39130109
I	19.07426676	-1.48759928	-1.94086236
C	8.54493840	-0.00327086	-0.13998035
O	16.11234260	-0.72487110	1.82665973
H	14.88637459	-1.71708214	2.54513564
O	14.14763953	-2.36959237	2.65306229
H	13.36735720	-1.85336841	2.88775124
H	14.61351633	-3.21574783	0.66634680

**d. Transition State 3**

C	2.17086817	1.20001432	-0.22223406
C	4.28742600	-0.00863885	-0.05784648
C	6.41586072	-1.23600124	-0.09076925
C	8.53970238	-2.45912078	-0.21175461
C	10.65122313	-3.71090567	-0.41825266
C	4.30231224	2.42609822	0.19758084
C	6.41282440	1.22843668	-0.06525243
C	9.96222426	-0.00754564	-0.15992863
C	10.66965171	-1.24269493	-0.25169102
C	12.76793642	-2.51005411	-0.24871309
C	6.42816048	3.66729300	-0.21347148
C	8.54679048	2.45635953	-0.06416767
C	10.67555396	1.21797626	-0.11752984
C	12.80819005	-0.02429599	-0.24710348
C	14.92719137	-1.24757687	-0.06529585
C	8.56856464	4.88639316	0.19608562
C	10.67940818	3.68145903	-0.06956348
C	12.81058081	2.44426577	-0.12229767
C	14.95232330	1.21799796	-0.09059213
C	17.10392430	-0.00391952	-0.09992470

C	3.56986580	1.23651936	-0.02352373
C	5.70529098	-0.00213096	-0.05257793
C	7.82971379	-1.22998360	-0.15031852
C	9.95799309	-2.46673503	-0.30158735
C	12.04717658	-3.70684070	-0.18876335
C	5.69453966	2.47372764	-0.02748434
C	7.83170878	1.23128379	-0.10524236
C	12.08531241	-1.25929263	-0.29112196
C	14.22953174	-2.51423256	-0.05794176
C	7.82897059	3.70217460	-0.02479462
C	9.96641650	2.45411381	-0.06320160
C	12.09842481	1.21131936	-0.16651459
C	14.23521528	-0.02542160	-0.17697725
C	16.29601326	-1.10403900	0.57810954
C	9.96183004	4.92740138	-0.03176263
C	12.09987255	3.68031215	-0.10312249
C	14.23800356	2.44367522	-0.10640537
C	16.37898787	1.23499564	-0.08291483
C	18.39524654	0.01355323	-0.57404696
I	17.56089353	-3.11917939	0.96630778
I	15.17639229	-3.65215918	-1.77412680
I	12.94599820	-5.42389868	0.70802950
I	7.70593673	6.40172157	1.43596999
I	5.53019439	5.23000541	-1.36925998
I	3.42272189	3.93490397	1.43348154
I	1.27595012	2.75306109	-1.39065144
I	19.07872715	-1.48513167	-1.93287760
C	8.54242075	-0.00178845	-0.13654125
O	16.02707622	-0.73921599	1.81605470
H	14.96977782	-1.68936837	2.43229639
O	14.31309989	-2.44470069	2.64873505
H	13.43159643	-2.04964888	2.72002541
H	14.41049077	-2.92791711	1.01715401



**e. Transition State 4**

C	2.16999701	1.20092989	-0.21966569
C	4.28674435	-0.00890541	-0.05796420
C	6.41538217	-1.23750458	-0.09174527
C	8.54006690	-2.46218726	-0.20972465
C	10.65236239	-3.71532849	-0.41813953
C	4.30233048	2.42591768	0.19591816
C	6.41335621	1.22758995	-0.06539142
C	9.96204831	-0.00814295	-0.15709784
C	10.67026472	-1.24452473	-0.24454685
C	12.77997191	-2.50887348	-0.26676195
C	6.42795459	3.66712531	-0.21137643
C	8.54674277	2.45579157	-0.06425189
C	10.67590177	1.21869927	-0.11799281
C	12.80891264	-0.02240369	-0.23698152
C	14.91679707	-1.26827740	-0.08058250
C	8.56860245	4.88649920	0.19491271
C	10.67960726	3.68186889	-0.07002965
C	12.80985632	2.44435460	-0.12255143
C	14.94929009	1.21319839	-0.07077737
C	17.09832205	-0.01030431	-0.07618830
C	3.56887714	1.23698124	-0.02418512
C	5.70476764	-0.00244847	-0.05379501
C	7.82986551	-1.23114167	-0.15001824
C	9.95760776	-2.46739455	-0.30116772
C	12.04603522	-3.71078864	-0.20598159
C	5.69462738	2.47380022	-0.02756441
C	7.83158089	1.23109964	-0.10544443
C	12.08683307	-1.25555415	-0.27625495
C	14.22836436	-2.47970400	-0.22503730
C	7.82867771	3.70228900	-0.02459664
C	9.96618693	2.45512370	-0.06396068
C	12.09661766	1.21595530	-0.16794833

C	14.22603106	-0.02310069	-0.13523025
C	16.28936714	-1.13024562	0.57360335
C	9.96079225	4.92860820	-0.03232280
C	12.09844220	3.68210765	-0.10272007
C	14.23586058	2.44297714	-0.10425308
C	16.37677185	1.23152555	-0.07228788
C	18.39099920	0.00619338	-0.56134317
I	17.54829990	-3.11028901	0.95992606
I	15.18370408	-3.69340531	-1.77021158
I	12.95544653	-5.42203092	0.70229436
I	7.70502701	6.40239711	1.43503197
I	5.52989053	5.23048789	-1.36797351
I	3.42272409	3.93509475	1.43298052
I	1.27557763	2.75437148	-1.38993733
I	19.07797012	-1.48536767	-1.92988524
C	8.54281064	-0.00311801	-0.13654023
O	15.97830544	-0.78811870	1.85126682
H	15.13595478	-1.58444350	2.32844550
O	14.31976064	-2.51112934	2.48510530
H	13.45241476	-2.09797229	2.67987871
H	14.33018413	-2.81348975	1.40620255

**f. Transition State 5**

C	2.17614739	1.20400648	-0.22254365
C	4.29526367	-0.00786092	-0.06257452
C	6.42846690	-1.24152946	-0.07732633
C	8.55991411	-2.46744545	-0.18485759
C	10.69054125	-3.70706839	-0.45747055
C	4.31211996	2.42576625	0.18507105
C	6.42406220	1.22386556	-0.07064605
C	9.97682316	-0.00966945	-0.12462295
C	10.69163073	-1.24554454	-0.22025092
C	12.82802007	-2.47128482	-0.45959621
C	6.43586278	3.66533984	-0.21831766

C	8.55497300	2.45478221	-0.06514124
C	10.68583257	1.22136505	-0.09731182
C	12.82019662	-0.00940926	-0.18216069
C	14.94221336	-1.27030020	-0.13124462
C	8.57471999	4.88757920	0.18353522
C	10.68723836	3.68424609	-0.07184206
C	12.81952369	2.44881981	-0.09187648
C	14.95975376	1.20816004	-0.00092200
C	17.12644878	-0.00549820	-0.13211862
C	3.57616490	1.23843461	-0.03314958
C	5.71500057	-0.00540475	-0.05576626
C	7.84566322	-1.23586492	-0.12356205
C	9.97979982	-2.47032309	-0.29056386
C	12.10404230	-3.68679324	-0.39243406
C	5.70479278	2.47080939	-0.03691559
C	7.84236862	1.22806706	-0.10117928
C	12.10945440	-1.23921183	-0.28751637
C	14.26192688	-2.38549764	-0.60016512
C	7.83586561	3.70157560	-0.03184605
C	9.97433063	2.45723563	-0.06080736
C	12.10642482	1.22361704	-0.12162232
C	14.23039363	-0.02307720	-0.06210548
C	16.33904903	-1.14885037	0.47531305
C	9.96777087	4.93104290	-0.04004506
C	12.10588141	3.68525965	-0.09751649
C	14.24543354	2.43994410	-0.06077499
C	16.39272642	1.22674606	-0.06299408
C	18.42939918	0.01646678	-0.59323152
I	17.44473562	-3.11475476	0.81138603
I	15.19508075	-3.67127829	-2.04037156
I	13.09078163	-5.39221195	0.46532451
I	7.70499139	6.40293582	1.42281712
I	5.53453226	5.22828723	-1.37438325

I	3.43713457	3.93553701	1.42735520
I	1.27934587	2.76539899	-1.38388721
I	19.07578796	-1.45983363	-2.00734801
C	8.55626227	-0.00682937	-0.11492365
O	16.16380337	-0.71543150	1.81272675
H	15.51889945	-1.33009741	2.24720921
O	14.03329579	-2.32122182	2.69826618
H	13.21766749	-1.84008296	2.91219290
H	13.85321961	-2.71294381	1.82699798

**g. Final**

C	2.18606378	1.20667350	-0.23041442
C	4.30499954	-0.00532906	-0.06392469
C	6.43922648	-1.24009627	-0.07579775
C	8.57226231	-2.47004466	-0.17612438
C	10.70770710	-3.70952971	-0.42792984
C	4.32249238	2.42989178	0.17357151
C	6.43479709	1.22544052	-0.07270109
C	9.98772403	-0.00904444	-0.12536096
C	10.70331337	-1.24507190	-0.22025983
C	12.84203804	-2.47047444	-0.44961033
C	6.44626640	3.66787808	-0.22858360
C	8.56468976	2.45679911	-0.06652978
C	10.69590023	1.22312884	-0.09761169
C	12.82951301	-0.00820737	-0.18822172
C	14.94718426	-1.27084456	-0.15085210
C	8.58423040	4.89112757	0.17482905
C	10.69718656	3.68636991	-0.07201362
C	12.82908070	2.45082645	-0.09272137
C	14.96837729	1.20910149	-0.00466566
C	17.13684655	-0.01293138	-0.10046105
C	3.58576853	1.24191990	-0.03991871
C	5.72508533	-0.00339665	-0.05561549
C	7.85720585	-1.23647515	-0.12151932

C	9.99283691	-2.47183730	-0.28191341
C	12.12206310	-3.68513877	-0.36092190
C	5.71577749	2.47295543	-0.04465929
C	7.85281867	1.22919148	-0.10157664
C	12.12185153	-1.23917306	-0.28835910
C	14.27030605	-2.39196615	-0.59254960
C	7.84552525	3.70465179	-0.03821968
C	9.98413196	2.45925630	-0.06013957
C	12.11659193	1.22504964	-0.12330352
C	14.23970616	-0.02140523	-0.07434470
C	16.32838943	-1.17126521	0.45960006
C	9.97813773	4.93349966	-0.04427235
C	12.11564503	3.68757517	-0.09728947
C	14.25488117	2.44206869	-0.06198940
C	16.40185132	1.22424850	-0.05230848
C	18.45307487	0.00496148	-0.53408705
I	17.43912066	-3.09904907	0.86236832
I	15.22161330	-3.72342934	-1.97913499
I	13.10168291	-5.35815497	0.55469264
I	7.70954294	6.41232270	1.40421241
I	5.54966698	5.22413040	-1.39774375
I	3.44387649	3.94837582	1.40322121
I	1.29020912	2.76042900	-1.40347148
I	19.11255163	-1.47936747	-1.94058674
C	8.56688754	-0.00640024	-0.11448147
O	15.98628086	-0.80123390	1.82345986
H	16.80618129	-0.80661447	2.35374556
O	13.62855712	-2.41985699	2.81692627
H	12.97739483	-1.75614533	3.08770627
H	14.34950930	-1.89292308	2.42137047

#### 4) HOH formation

##### a. Initial

C	2.18582126	1.19960788	-0.22385424
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C	4.30435567	-0.01075052	-0.06584154
C	6.43752080	-1.23740166	-0.09513286
C	8.57040844	-2.46282873	-0.20372032
C	10.69822398	-3.71282869	-0.31814273
C	4.32026824	2.42147091	0.19750084
C	6.43281357	1.22557780	-0.06864966
C	9.98805251	-0.00916228	-0.18982319
C	10.70342548	-1.24271983	-0.25920303
C	12.82453284	-2.49460359	-0.26495121
C	6.44529507	3.66350855	-0.21484712
C	8.56667742	2.45260051	-0.07268404
C	10.70317201	1.21770946	-0.16023067
C	12.83580209	-0.02037136	-0.29943339
C	14.95245929	-1.24375974	-0.10028785
C	8.58633636	4.88211167	0.19362121
C	10.69788721	3.68021994	-0.08261783
C	12.83062801	2.44414156	-0.15518560
C	14.97223958	1.21873396	-0.10513691
C	17.12267794	-0.00540570	-0.09314624
C	3.58454739	1.23517723	-0.02825582
C	5.72426965	-0.00444555	-0.05692617
C	7.85553677	-1.23389789	-0.15446340
C	9.99100102	-2.46953744	-0.26490944
C	12.10260574	-3.68586512	-0.13790441
C	5.71290698	2.47094119	-0.02854843
C	7.85212799	1.22686535	-0.11212166
C	12.12301099	-1.25247416	-0.32282364
C	14.27903077	-2.48564461	-0.21828408
C	7.84586810	3.69926214	-0.02841101
C	9.98820512	2.45157129	-0.08047316
C	12.12637330	1.20956738	-0.22106957
C	14.26733140	-0.02734566	-0.22189318
C	16.31804746	-1.14029522	0.50773318

C	9.97894781	4.92597262	-0.03691336
C	12.11870621	3.67707843	-0.12018911
C	14.25712252	2.44350047	-0.11864868
C	16.39719041	1.23192413	-0.09031435
C	18.45399072	0.00713438	-0.47441678
I	17.44199710	-3.08829322	0.85158137
I	15.17106083	-3.83076626	-2.10043565
I	13.04529324	-5.39219656	0.73426321
I	7.72506698	6.39296162	1.43752481
I	5.54569638	5.22515046	-1.36631817
I	3.44335476	3.92634493	1.43741455
I	1.29102252	2.75205878	-1.38907206
I	19.15452563	-1.44741351	-1.88392156
C	8.56533986	-0.00544071	-0.14944247
O	16.05926160	-0.75217412	1.87426401
H	16.90840072	-0.74313586	2.35857652
H	14.45090636	-1.67948117	2.56026978
O	13.74022198	-2.34587091	2.62781957
H	13.11093143	-1.99112914	3.27046275
H	14.68650505	-3.25965339	0.43913537

**b. Transition State 1**

C	2.17716165	1.19479608	-0.22790923
C	4.29577963	-0.01426431	-0.06402001
C	6.42832639	-1.24027307	-0.07978874
C	8.55906290	-2.46278143	-0.18637805
C	10.68428227	-3.70629584	-0.37116287
C	4.31125298	2.41736754	0.18344404
C	6.42350806	1.22092940	-0.06824149
C	9.97778882	-0.01187928	-0.14923279
C	10.69054108	-1.24343731	-0.24902484
C	12.80881612	-2.49145464	-0.33086231
C	6.43693764	3.65833366	-0.22382339
C	8.55690881	2.44820323	-0.06724755

C	10.68935891	1.21546357	-0.11871818
C	12.82129718	-0.01370317	-0.31193569
C	14.95566368	-1.22707460	-0.20090162
C	8.57587071	4.87734062	0.18287126
C	10.68765971	3.67690974	-0.07550068
C	12.82079687	2.44514467	-0.12468323
C	14.96247856	1.22221056	-0.12697296
C	17.10939126	0.00120980	-0.18347347
C	3.57600390	1.23034583	-0.03587324
C	5.71517169	-0.00854665	-0.05079046
C	7.84629823	-1.23685408	-0.12165102
C	9.97889925	-2.46925240	-0.25975671
C	12.09370086	-3.68279683	-0.20083455
C	5.70367415	2.46625140	-0.03966651
C	7.84267002	1.22331607	-0.09967957
C	12.10749760	-1.24710456	-0.36652418
C	14.26975633	-2.48400233	-0.28166092
C	7.83659127	3.69383631	-0.03606016
C	9.97684221	2.44873970	-0.06318272
C	12.11229006	1.21204541	-0.18543830
C	14.25580943	-0.01543770	-0.26954537
C	16.32268358	-1.13722120	0.32300035
C	9.96881592	4.92211175	-0.04279444
C	12.10838985	3.67595602	-0.10525131
C	14.24720132	2.44346650	-0.10492212
C	16.38582570	1.23400000	-0.12442694
C	18.44604959	0.02642618	-0.57801820
I	17.41073412	-2.97116690	0.76776270
I	15.14288085	-3.83412396	-2.09069395
I	13.02730122	-5.38773069	0.67772778
I	7.71149988	6.38547808	1.42790680
I	5.53885740	5.21754044	-1.38069968
I	3.43835459	3.92215111	1.42692358



I	1.28016331	2.74848308	-1.39175065
I	19.17855495	-1.35639843	-2.04163881
C	8.55640124	-0.00830107	-0.11393924
O	15.99110203	-0.56856584	1.99433596
H	16.70468430	-0.87822192	2.58835241
H	14.82519540	-1.63620709	2.40671659
O	14.23692894	-2.41932235	2.62099730
H	13.34141493	-2.06461615	2.56638341
H	14.61950868	-3.16000159	0.49871652

**c. Transition State 2**

C	2.17653354	1.19490442	-0.22927667
C	4.29531712	-0.01509315	-0.06430501
C	6.42634076	-1.24300356	-0.07588960
C	8.55509054	-2.46931175	-0.17669901
C	10.68234076	-3.70844312	-0.36317987
C	4.31030112	2.41793240	0.18391658
C	6.42264944	1.21963252	-0.06877986
C	9.97458672	-0.01238018	-0.13942775
C	10.68367674	-1.24427853	-0.23597087
C	12.79713329	-2.48887035	-0.37801305
C	6.43638419	3.65812719	-0.22492560
C	8.55608637	2.44654742	-0.06773943
C	10.68830950	1.21429249	-0.11154465
C	12.82142131	-0.01543670	-0.29900084
C	14.97283454	-1.22512064	-0.28157323
C	8.57497726	4.87743100	0.18300506
C	10.68744927	3.67591648	-0.07514273
C	12.82093601	2.44372241	-0.11686430
C	14.95919282	1.21659633	-0.13493825
C	17.09863608	-0.01082895	-0.24706946
C	3.57508864	1.23086932	-0.03632714
C	5.71401159	-0.00938439	-0.05073919
C	7.84441631	-1.24026147	-0.11383005

C	9.97314446	-2.47162488	-0.24927564
C	12.09344656	-3.67901229	-0.21963655
C	5.70305899	2.46571906	-0.03999970
C	7.84144593	1.22158688	-0.09934549
C	12.09628194	-1.24663988	-0.35687909
C	14.26048189	-2.48236004	-0.34503777
C	7.83610838	3.69309197	-0.03660114
C	9.97620468	2.44771748	-0.06219223
C	12.11180064	1.21118054	-0.16950562
C	14.25387997	-0.00933911	-0.28775750
C	16.34788014	-1.19809376	0.03008346
C	9.96822288	4.92172703	-0.04369708
C	12.10727530	3.67677815	-0.10339000
C	14.24373996	2.44353839	-0.09837990
C	16.37850510	1.22396614	-0.14191474
C	18.45388154	0.03287965	-0.59772344
I	17.38498147	-2.94634329	0.71053057
I	15.11470087	-3.83748165	-2.08095224
I	13.02917984	-5.37705251	0.67121791
I	7.71160032	6.38356481	1.42875838
I	5.53854456	5.21689567	-1.38085958
I	3.43798956	3.92340566	1.42692346
I	1.27925299	2.74849462	-1.39162045
I	19.20088724	-1.33349948	-2.06829553
C	8.55406474	-0.01036937	-0.10892921
O	15.90852764	-0.47318494	2.24878651
H	16.66753080	-0.85926601	2.72556667
H	14.89410784	-1.57855370	2.39881897
O	14.27456974	-2.41302613	2.45712704
H	13.37877900	-2.06631875	2.55869679
H	14.57264552	-3.07421573	0.52964809

**d. Transition State 3**

C	2.17545963	1.19529666	-0.22796180
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C	4.29481274	-0.01576365	-0.06431090
C	6.42494463	-1.24555772	-0.07214971
C	8.55367057	-2.47431469	-0.16339844
C	10.68096267	-3.70895519	-0.35916898
C	4.30969110	2.41801386	0.18113327
C	6.42233514	1.21848974	-0.06903452
C	9.97330639	-0.01450771	-0.13216753
C	10.68192226	-1.24622247	-0.22823094
C	12.78969639	-2.48728106	-0.41660068
C	6.43581707	3.65812141	-0.22446846
C	8.55553819	2.44499383	-0.06805489
C	10.68758587	1.21257384	-0.10601241
C	12.82156834	-0.01572576	-0.29961197
C	14.97716620	-1.22484919	-0.38304765
C	8.57424946	4.87695672	0.18037886
C	10.68720183	3.67490765	-0.07492978
C	12.82019109	2.44281745	-0.11182198
C	14.95581881	1.21116598	-0.14185736
C	17.09313970	-0.01532056	-0.28582858
C	3.57394675	1.23130891	-0.03715869
C	5.71326183	-0.01085068	-0.05069386
C	7.84389416	-1.24356266	-0.10643672
C	9.97047435	-2.47386344	-0.23887427
C	12.09383939	-3.67696422	-0.23495532
C	5.70252968	2.46565886	-0.04109810
C	7.84076927	1.22073804	-0.09841504
C	12.09329328	-1.24654711	-0.35987586
C	14.25120745	-2.48071776	-0.40841461
C	7.83537158	3.69251338	-0.03757496
C	9.97570464	2.44649842	-0.06109629
C	12.11065935	1.21081384	-0.16021719
C	14.25050792	-0.00624202	-0.31617184
C	16.35298394	-1.22185145	-0.15751169

C	9.96765709	4.92146917	-0.04507077
C	12.10639179	3.67694101	-0.10160558
C	14.24157046	2.44189987	-0.09245540
C	16.37598214	1.21689356	-0.14496931
C	18.45911458	0.03792205	-0.60885411
I	17.36884494	-2.92785617	0.64688491
I	15.08652088	-3.84083935	-2.07121053
I	13.03243824	-5.36925880	0.66558078
I	7.71163949	6.38215982	1.42891118
I	5.53840739	5.21726063	-1.38092929
I	3.43881477	3.92277310	1.42475544
I	1.27766140	2.74970706	-1.39034254
I	19.22017723	-1.31226839	-2.09140291
C	8.55330940	-0.01344572	-0.10509451
O	15.79660780	-0.51584300	2.46228241
H	16.65335004	-0.88077142	2.74088306
H	15.03003287	-1.47642801	2.38617672
O	14.30018463	-2.41061008	2.29312571
H	13.41380485	-2.09277570	2.52499962
H	14.50704648	-2.95081075	0.59644746

**e. Transition State 4**

C	2.17571129	1.19484027	-0.22826606
C	4.29466510	-0.01643612	-0.06481844
C	6.42553484	-1.24732816	-0.07275226
C	8.55465871	-2.47705810	-0.16461658
C	10.68485002	-3.71368808	-0.36240630
C	4.30987312	2.41721596	0.18116970
C	6.42284305	1.21688681	-0.06984936
C	9.97382748	-0.01535176	-0.13253132
C	10.68348896	-1.24875490	-0.22623211
C	12.80021934	-2.49254362	-0.42478016
C	6.43590319	3.65723763	-0.22420507
C	8.55600614	2.44362073	-0.06855238

C	10.68861272	1.21205732	-0.10703076
C	12.82294790	-0.01924775	-0.29407448
C	14.97238022	-1.24551382	-0.38491096
C	8.57461131	4.87603255	0.18028313
C	10.68780119	3.67414583	-0.07521448
C	12.82033606	2.44127940	-0.11246797
C	14.95653680	1.20672920	-0.13603941
C	17.09186164	-0.02306285	-0.28965022
C	3.57449510	1.22997940	-0.03747571
C	5.71324133	-0.01178900	-0.05173183
C	7.84405820	-1.24484104	-0.10610338
C	9.97102026	-2.47456185	-0.24015784
C	12.09120968	-3.68420656	-0.24234192
C	5.70295885	2.46410234	-0.04133348
C	7.84086812	1.21956315	-0.09931417
C	12.09584900	-1.24768543	-0.35309826
C	14.24193301	-2.47907547	-0.47179145
C	7.83587309	3.69098277	-0.03781759
C	9.97579245	2.44643679	-0.06158330
C	12.11002155	1.21147938	-0.16159033
C	14.24892842	-0.01246066	-0.29704705
C	16.35754248	-1.22876335	-0.17014893
C	9.96778606	4.92143624	-0.04546617
C	12.10645853	3.67653829	-0.10153707
C	14.24182743	2.44007295	-0.09206492
C	16.37487985	1.21432516	-0.14736057
C	18.45998579	0.03419018	-0.60694100
I	17.37219070	-2.93336689	0.64483510
I	15.05834090	-3.84419704	-2.06146883
I	13.02961503	-5.37699277	0.66228132
I	7.71318257	6.37989249	1.43001497
I	5.53827714	5.21709920	-1.37964144
I	3.43887844	3.92254808	1.42421307

I	1.27781571	2.74994648	-1.38927865
I	19.21989323	-1.31357804	-2.09407255
C	8.55416772	-0.01490233	-0.10566131
O	15.76631729	-0.53860294	2.46887278
H	16.63377252	-0.88429260	2.73747013
H	15.13609293	-1.39723268	2.38542663
O	14.30292564	-2.52524477	2.16515571
H	13.43572768	-2.15257016	2.43044376
H	14.41153089	-2.82834032	0.91173829

**f. Transition State 5**

C	2.17781355	1.18724004	-0.22465236
C	4.29816478	-0.02896072	-0.06896505
C	6.43018127	-1.26550840	-0.07408801
C	8.56119197	-2.50101109	-0.16370004
C	10.69689779	-3.74238643	-0.33774971
C	4.31282528	2.40739574	0.17742347
C	6.42643758	1.20348670	-0.07432589
C	9.98019008	-0.03322741	-0.11417912
C	10.69319967	-1.27089369	-0.17610302
C	12.82637339	-2.52344677	-0.35526638
C	6.43811730	3.64821420	-0.21993589
C	8.55865588	2.43265944	-0.07063075
C	10.69224385	1.19786818	-0.09962882
C	12.82836819	-0.04167971	-0.24395268
C	14.97036084	-1.28643223	-0.33655783
C	8.57627773	4.86755535	0.17617171
C	10.69014827	3.66364018	-0.07851030
C	12.82440276	2.42619645	-0.11033759
C	14.96220747	1.18102480	-0.11925058
C	17.09713546	-0.05756966	-0.30755601
C	3.57696875	1.22048849	-0.03941011
C	5.71704875	-0.02654186	-0.05600123
C	7.85022133	-1.26459422	-0.10248385

C	9.98049960	-2.49872471	-0.21864145
C	12.10002437	-3.72163210	-0.20979128
C	5.70611291	2.45357105	-0.04412323
C	7.84466086	1.20643233	-0.10217285
C	12.11049128	-1.27054159	-0.26740581
C	14.23265857	-2.47743319	-0.53516830
C	7.83804114	3.68150219	-0.03843364
C	9.97838997	2.43556560	-0.06310722
C	12.11330282	1.19672472	-0.14545665
C	14.24929130	-0.04051614	-0.23975780
C	16.37069968	-1.26047902	-0.19660166
C	9.96939013	4.91308305	-0.04824373
C	12.10895404	3.66484787	-0.10446031
C	14.24684198	2.41984805	-0.08730621
C	16.38095446	1.18497026	-0.16174238
C	18.47386465	0.00615985	-0.60169820
I	17.36632958	-2.96003128	0.65396820
I	15.03016092	-3.84755474	-2.05172712
I	13.04807670	-5.42255624	0.67520895
I	7.71313513	6.37494524	1.42660027
I	5.53850303	5.21209670	-1.37351258
I	3.44301899	3.91223857	1.42670391
I	1.27934706	2.74772561	-1.38403272
I	19.23849888	-1.33249070	-2.09256177
C	8.55902543	-0.03146252	-0.10340177
O	15.84187732	-0.47532310	2.47652846
H	16.68332914	-0.87207748	2.74084451
H	15.20141804	-1.22814884	2.54383753
O	14.10032587	-2.53860238	2.46905027
H	13.23022833	-2.12046526	2.54458815
H	14.18491133	-2.74799367	1.51063311

**g. Final**

C	2.17590793	1.17209225	-0.22392465
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C	4.29708109	-0.04429260	-0.07337341
C	6.43097056	-1.28434096	-0.07098688
C	8.56496486	-2.52487666	-0.12782347
C	10.70288735	-3.76486808	-0.28773218
C	4.31152239	2.39291824	0.17221530
C	6.42632327	1.18552255	-0.07938267
C	9.98423399	-0.05595731	-0.07419882
C	10.70087481	-1.29685855	-0.09546730
C	12.83731598	-2.53857962	-0.31504258
C	6.43729625	3.63219629	-0.22438430
C	8.55836105	2.41589223	-0.07365770
C	10.69295826	1.17716972	-0.07383192
C	12.82914249	-0.06166184	-0.15230508
C	14.96789201	-1.30577275	-0.31668209
C	8.57328596	4.85304812	0.17192191
C	10.68827789	3.64613441	-0.07975769
C	12.82387777	2.40902574	-0.09225287
C	14.96269760	1.16082947	-0.09100379
C	17.09856464	-0.07783800	-0.28783579
C	3.57571712	1.20576254	-0.04343462
C	5.71640217	-0.04434870	-0.05858739
C	7.85212931	-1.28546840	-0.08905411
C	9.98513513	-2.52259055	-0.15197177
C	12.10887109	-3.73923619	-0.17835987
C	5.70548864	2.43649515	-0.05134244
C	7.84560505	1.18837418	-0.10380183
C	12.11971123	-1.29315457	-0.17612670
C	14.22338413	-2.47579090	-0.59854514
C	7.83715366	3.66598164	-0.04367519
C	9.97781680	2.41680894	-0.05948846
C	12.11467537	1.17611108	-0.09633773
C	14.24968957	-0.06348533	-0.17291113
C	16.37041313	-1.27998039	-0.19029551



C	9.96704716	4.89688677	-0.05156870
C	12.10775865	3.64879716	-0.10401347
C	14.24650159	2.40171807	-0.07288863
C	16.38076383	1.16430205	-0.14471228
C	18.48232878	-0.01511690	-0.56232551
I	17.33576284	-2.97686534	0.69914943
I	15.00198094	-3.85091243	-2.04198541
I	13.07812426	-5.42120041	0.73680137
I	7.70678406	6.35816732	1.42265957
I	5.53600844	5.19672510	-1.37744776
I	3.44570127	3.89726019	1.42423481
I	1.27491966	2.73704743	-1.37700531
I	19.27895891	-1.37280786	-2.01811937
C	8.56142455	-0.05153552	-0.09015768
O	15.89235346	-0.44759873	2.64348167
H	16.70717955	-0.89628921	2.90885201
H	15.19992235	-1.14130777	2.72217334
O	13.78213262	-2.30783513	2.72696338
H	12.95522811	-1.93839281	3.07164027
H	13.55131702	-2.70535328	1.87069616

## 5) HOOH formation

### a. Initial

C	2.20277537	1.20743997	-0.24463920
C	4.32111525	-0.00139672	-0.06676074
C	6.45502081	-1.23249892	-0.08346266
C	8.58704580	-2.46332732	-0.19030847
C	10.71155609	-3.72078108	-0.35960820
C	4.33719090	2.43212694	0.17382774
C	6.44995921	1.23175815	-0.07126559
C	10.00194906	-0.00535292	-0.15132212
C	10.71513161	-1.24188081	-0.23202066
C	12.83727598	-2.49061388	-0.26198996
C	6.46189087	3.67176726	-0.23892332

C	8.58118344	2.46130217	-0.07088999
C	10.71430833	1.22439002	-0.11687681
C	12.84528199	-0.01342809	-0.23237112
C	14.95374864	-1.24445661	-0.03118785
C	8.60129534	4.89288533	0.17337478
C	10.71394564	3.68773140	-0.07597299
C	12.84632717	2.45369136	-0.11070610
C	14.98445285	1.22213480	-0.05149938
C	17.13599281	-0.00604746	-0.10198570
C	3.60102617	1.24537892	-0.04511087
C	5.74119249	0.00169007	-0.05414417
C	7.87399839	-1.23209200	-0.13670542
C	10.00666393	-2.47258621	-0.26376821
C	12.11994125	-3.69132901	-0.20257665
C	5.73079119	2.47817864	-0.04508929
C	7.86889045	1.23377061	-0.10481687
C	12.13370456	-1.24623412	-0.28030364
C	14.29546501	-2.48851537	-0.25129398
C	7.86074258	3.70962597	-0.04397786
C	10.00177557	2.45984080	-0.06466019
C	12.13859074	1.21894964	-0.15752108
C	14.27144952	-0.02198706	-0.12322225
C	16.34671095	-1.14185323	0.50594457
C	9.99558351	4.93411751	-0.04817432
C	12.13486828	3.68698383	-0.10434301
C	14.27329566	2.44878722	-0.08426630
C	16.41156145	1.23073200	-0.07257557
C	18.45783244	0.00505253	-0.51948285
I	17.42939932	-3.13487408	0.77005042
I	15.05170290	-3.29165303	-2.46272675
I	13.14560915	-5.44696493	0.46618323
I	7.73011001	6.41732785	1.39401702
I	5.56805617	5.21894566	-1.41360301

I	3.45343480	3.94993376	1.39358376
I	1.31373427	2.74622680	-1.43248225
I	19.09671424	-1.43574087	-1.96681330
C	8.58135790	-0.00034175	-0.12635466
O	16.04764245	-0.77662642	1.86800649
O	17.27011336	-0.39972626	2.64279887
H	17.58097662	-1.29926913	2.89477134
H	14.16882770	-1.24053049	3.41126870
O	13.41897464	-1.78750362	3.12904529
H	12.74400022	-1.66991926	3.81128808
H	14.74558951	-3.33948273	0.25931616

**b. Transition State 1**

C	2.20888016	1.19150449	-0.28016108
C	4.32674613	-0.01623706	-0.07795298
C	6.45928498	-1.24534161	-0.07564968
C	8.59027404	-2.47895508	-0.16016443
C	10.71963636	-3.72795523	-0.30445271
C	4.33810000	2.42075962	0.14302046
C	6.45400654	1.21905010	-0.07753426
C	10.00415670	-0.01560365	-0.12890202
C	10.71383559	-1.25121938	-0.20353404
C	12.83188671	-2.49228351	-0.26823424
C	6.46677577	3.65776652	-0.26839091
C	8.58602692	2.44719707	-0.07891452
C	10.71891837	1.21290969	-0.10925374
C	12.85163259	-0.02297148	-0.25526888
C	14.98606533	-1.24285385	-0.14935836
C	8.60398527	4.88180177	0.14233458
C	10.71969819	3.67468085	-0.08513931
C	12.85343146	2.44147222	-0.11613536
C	14.99057302	1.20812996	-0.10512141
C	17.13179889	-0.03171334	-0.17775184
C	3.60655214	1.23007902	-0.07237029

C	5.74581504	-0.01067898	-0.05458686
C	7.87852660	-1.24642614	-0.11107641
C	10.00862630	-2.48431470	-0.22089483
C	12.12921976	-3.69109703	-0.16204153
C	5.73422655	2.46521984	-0.06809980
C	7.87226688	1.22101728	-0.10333792
C	12.12964359	-1.25201856	-0.28318114
C	14.28566605	-2.48736684	-0.31684813
C	7.86609481	3.69464380	-0.06839968
C	10.00648817	2.44784278	-0.06589377
C	12.14417375	1.20827824	-0.15970453
C	14.28151586	-0.02242436	-0.21520847
C	16.37234085	-1.21172002	0.13735678
C	10.00038564	4.92008172	-0.07423206
C	12.14005496	3.67422746	-0.11026093
C	14.27720667	2.43897040	-0.09430515
C	16.41096851	1.21241309	-0.10925811
C	18.48795116	0.00367778	-0.51352902
I	17.38129063	-3.02009962	0.72080246
I	15.03217645	-3.39282999	-2.40114031
I	13.15250756	-5.42295218	0.55673432
I	7.72863806	6.41347982	1.34857303
I	5.57997565	5.19456971	-1.46069531
I	3.44825625	3.94554555	1.34771713
I	1.32392161	2.72050399	-1.48325873
I	19.19440342	-1.37395599	-2.00068623
C	8.58399387	-0.01288687	-0.10760175
O	16.02711723	-0.57947900	2.20689735
O	17.26291410	-0.41426171	2.84093871
H	17.47850487	-1.33664087	3.10502414
H	14.63777859	-1.58043228	2.82140489
O	13.84612413	-2.14492708	2.98970375
H	13.09997668	-1.53222897	3.04526775

H 14.72238070 -3.29404812 0.27591352

**c. Transition State 2**

C	2.20156541	1.19481062	-0.27600738
C	4.31924589	-0.01319564	-0.07597399
C	6.45130352	-1.23950826	-0.07492620
C	8.58251637	-2.47218298	-0.17162512
C	10.71026863	-3.72291199	-0.33362082
C	4.33172717	2.42412288	0.13609162
C	6.44760388	1.22198895	-0.07674770
C	9.99743146	-0.01239946	-0.12268653
C	10.70745422	-1.24749897	-0.20218462
C	12.81827988	-2.48910821	-0.31185044
C	6.46097438	3.65993411	-0.26819839
C	8.57972283	2.44889203	-0.07750942
C	10.71168758	1.21551809	-0.10230384
C	12.84473593	-0.01588523	-0.27062547
C	14.99132868	-1.22272206	-0.26785248
C	8.59665254	4.88420083	0.13599261
C	10.71215143	3.67774212	-0.08315466
C	12.84459482	2.44607747	-0.11232368
C	14.97926856	1.21974720	-0.14565060
C	17.11677130	-0.01575364	-0.27093732
C	3.59851144	1.23434741	-0.07247914
C	5.73812630	-0.00584096	-0.05317112
C	7.87038533	-1.24089167	-0.11006915
C	9.99925632	-2.47910673	-0.22505626
C	12.12301980	-3.68605226	-0.19167797
C	5.72741526	2.46906589	-0.07059614
C	7.86537951	1.22400514	-0.10035488
C	12.12089887	-1.24736283	-0.30264652
C	14.27586708	-2.48621831	-0.38240228
C	7.85951316	3.69716986	-0.06998900
C	9.99949385	2.45069139	-0.06320055

C	12.13563472	1.21341176	-0.15475092
C	14.27178732	-0.00134527	-0.27469390
C	16.36995191	-1.21089417	-0.08803135
C	9.99265863	4.92393565	-0.07506796
C	12.13090984	3.67985293	-0.10568618
C	14.26538657	2.44953507	-0.09862601
C	16.40003391	1.22191503	-0.15702576
C	18.48387623	0.02759159	-0.59249813
I	17.36484028	-2.95921140	0.64437834
I	15.01265001	-3.49400696	-2.33955387
I	13.13317614	-5.41503334	0.54538882
I	7.71770256	6.41790776	1.34114284
I	5.57362132	5.19632121	-1.46466796
I	3.44335584	3.95108425	1.34237548
I	1.31547168	2.72614663	-1.47892266
I	19.21595168	-1.32661123	-2.08681113
C	8.57768702	-0.01025453	-0.10281601
O	15.85604149	-0.30441829	2.40845134
O	17.09857134	-0.47005674	3.01177691
H	17.18971192	-1.44834984	3.09386330
H	14.78926546	-1.59904011	2.55944409
O	14.12995992	-2.34343122	2.63060432
H	13.26674665	-1.91710261	2.63066476
H	14.66503762	-3.18770592	0.36612426

**d. Transition State 3**

C	2.20017440	1.19000098	-0.27744253
C	4.31795961	-0.01844035	-0.07581716
C	6.44941213	-1.24609277	-0.06977578
C	8.57946789	-2.47736252	-0.17892821
C	10.70228796	-3.71725505	-0.38795685
C	4.33000930	2.41928142	0.13263555
C	6.44612602	1.21615689	-0.07738877
C	9.99566725	-0.01619664	-0.12018913

C	10.70551271	-1.24863145	-0.21932550
C	12.80621688	-2.48554755	-0.42716240
C	6.45942791	3.65440152	-0.27032091
C	8.57802349	2.44372069	-0.07730193
C	10.71032410	1.21158863	-0.09813094
C	12.84494463	-0.01680185	-0.28646556
C	14.99313601	-1.22315186	-0.38993820
C	8.59440520	4.88012197	0.13296142
C	10.71076566	3.67303284	-0.08257699
C	12.84363278	2.44129243	-0.10710188
C	14.97927509	1.21274176	-0.15508982
C	17.11674276	-0.02354162	-0.31502576
C	3.59710923	1.22903029	-0.07446204
C	5.73657507	-0.01169182	-0.05133468
C	7.86828010	-1.24675632	-0.10535184
C	9.99467400	-2.47768558	-0.24878599
C	12.11407068	-3.68112714	-0.27414238
C	5.72611865	2.46294893	-0.07364383
C	7.86362413	1.21901168	-0.09916722
C	12.11779890	-1.24540615	-0.35076207
C	14.26606812	-2.48506978	-0.44795643
C	7.85763102	3.69187836	-0.07192092
C	9.99779114	2.44636061	-0.06110347
C	12.13436220	1.20991891	-0.14926192
C	14.27086166	-0.00375832	-0.31027655
C	16.36997988	-1.22483280	-0.19291728
C	9.99086866	4.91933658	-0.07715772
C	12.12936785	3.67514702	-0.10363455
C	14.26481289	2.44238680	-0.09350131
C	16.40046906	1.21301974	-0.17867825
C	18.48181387	0.02875078	-0.63435294
I	17.36325629	-2.96909726	0.55837891
I	14.99312356	-3.59518392	-2.27796743

I	13.10922588	-5.39903556	0.52481440
I	7.71602640	6.41383576	1.33826585
I	5.57161314	5.19223322	-1.46505488
I	3.44343031	3.94681633	1.34059654
I	1.31380302	2.72398470	-1.47753255
I	19.22375844	-1.30864734	-2.14285266
C	8.57597882	-0.01538294	-0.09866635
O	15.73478151	-0.35594166	2.42988755
O	17.00040341	-0.52714605	3.01240490
H	17.10906080	-1.50482652	3.07327785
H	14.95478179	-1.55839419	2.38364051
O	14.36418312	-2.43455576	2.28136235
H	13.43722449	-2.16661053	2.36256323
H	14.49614086	-2.89580497	0.63946913

**e. Transition State 4**

C	2.20016420	1.19036112	-0.27653694
C	4.31794743	-0.01854074	-0.07574781
C	6.44925776	-1.24869208	-0.07007462
C	8.57943660	-2.48027794	-0.18050286
C	10.70518417	-3.72088584	-0.39037874
C	4.33020961	2.41947028	0.13312782
C	6.44643476	1.21517293	-0.07764201
C	9.99617820	-0.01715240	-0.11987161
C	10.70646922	-1.25186381	-0.21269201
C	12.82388129	-2.49218157	-0.42379949
C	6.45945725	3.65428455	-0.26947655
C	8.57798872	2.44318269	-0.07730586
C	10.71117625	1.21152317	-0.09864016
C	12.84547411	-0.02034019	-0.27795220
C	14.98390976	-1.25335131	-0.39049182
C	8.59456103	4.87983845	0.13328525
C	10.71085459	3.67285643	-0.08249362
C	12.84321382	2.43991482	-0.10793285



C	14.97915756	1.20554649	-0.15075449
C	17.11360332	-0.03151541	-0.31838640
C	3.59718532	1.22928894	-0.07416230
C	5.73640755	-0.01253405	-0.05210925
C	7.86830613	-1.24807861	-0.10475961
C	9.99511752	-2.47847226	-0.25014921
C	12.11156920	-3.69060614	-0.28013044
C	5.72637591	2.46233739	-0.07348762
C	7.86376817	1.21872519	-0.09951716
C	12.12106411	-1.24797440	-0.32633430
C	14.25626916	-2.48392125	-0.51351058
C	7.85762771	3.69171561	-0.07168059
C	9.99761877	2.44692526	-0.06120978
C	12.13301734	1.21131808	-0.15082758
C	14.26719932	-0.01364443	-0.29177450
C	16.37393717	-1.23120780	-0.20394558
C	9.99062245	4.91987100	-0.07723626
C	12.12894249	3.67546004	-0.10316028
C	14.26470977	2.43915549	-0.09364086
C	16.39941914	1.20982278	-0.18176254
C	18.48269300	0.02513954	-0.63384437
I	17.36513560	-2.97317214	0.55588280
I	14.97359712	-3.69636088	-2.21638099
I	13.10456142	-5.40605498	0.52850230
I	7.71578081	6.41428477	1.33817893
I	5.57159160	5.19246483	-1.46465897
I	3.44328867	3.94738491	1.34029786
I	1.31363909	2.72465638	-1.47697828
I	19.22335850	-1.30901190	-2.14482984
C	8.57651134	-0.01664406	-0.09923758
O	15.64262923	-0.42371799	2.44252561
O	16.97903372	-0.54058437	3.01225586
H	17.11639667	-1.50934065	3.07011876

H	15.12931452	-1.40674696	2.39253079
O	14.34876660	-2.52639019	2.13950018
H	13.44224154	-2.20614200	2.32011484
H	14.41627300	-2.78225322	1.04193678

**f. Transition State 5**

C	2.20700716	1.16567292	-0.28461953
C	4.32578338	-0.04714372	-0.08119984
C	6.45931453	-1.28567116	-0.06505992
C	8.59045198	-2.52532884	-0.13950543
C	10.72304634	-3.76486863	-0.31804506
C	4.33707592	2.39380088	0.12061363
C	6.45548125	1.18435608	-0.08347913
C	10.00797700	-0.05486281	-0.08388346
C	10.72068518	-1.29441085	-0.12073250
C	12.85221617	-2.53490033	-0.33202447
C	6.46788495	3.62592728	-0.28376606
C	8.58632466	2.41295355	-0.08221118
C	10.71968217	1.17735756	-0.08064431
C	12.85280496	-0.05700363	-0.22108628
C	14.98780802	-1.30154174	-0.35238769
C	8.59936407	4.85326940	0.12108238
C	10.71806653	3.64511004	-0.08635583
C	12.85172836	2.40809851	-0.10202971
C	14.98688198	1.16322170	-0.11962857
C	17.12187037	-0.07878840	-0.32941109
C	3.60489072	1.20163950	-0.08274078
C	5.74532928	-0.04552921	-0.05317125
C	7.87935743	-1.28656179	-0.08829567
C	10.00785666	-2.52254611	-0.17466727
C	12.12633951	-3.73451035	-0.19864415
C	5.73536019	2.43390335	-0.08402389
C	7.87397654	1.18552925	-0.10461846
C	12.13740179	-1.28665899	-0.22572603

C	14.24647020	-2.48277271	-0.57906473
C	7.86538565	3.66239005	-0.08275660
C	10.00602865	2.41638525	-0.05862361
C	12.14076896	1.17833737	-0.12296578
C	14.27170984	-0.05702512	-0.23144581
C	16.38832735	-1.27826433	-0.23836802
C	9.99748004	4.89381998	-0.08537307
C	12.13701276	3.64618887	-0.10740076
C	14.27280681	2.40232687	-0.08210273
C	16.40558459	1.16379979	-0.16963429
C	18.50409209	-0.01276476	-0.60498142
I	17.34405957	-3.00617731	0.60450166
I	14.95407067	-3.79753785	-2.15479456
I	13.11788476	-5.42075486	0.67130437
I	7.71941240	6.38406215	1.32969508
I	5.57903782	5.16871898	-1.47167754
I	3.45419755	3.92153284	1.33120233
I	1.32020266	2.70622045	-1.47511144
I	19.29245855	-1.35468065	-2.07865020
C	8.58755401	-0.05315613	-0.08922278
O	15.79093537	-0.50349632	2.43680166
O	17.04379535	-0.51775431	3.21060691
H	17.45804221	-1.34003030	2.87133993
H	15.21916643	-1.19329845	2.86949421
O	13.89485525	-2.33080705	2.68538625
H	13.02052985	-1.91631982	2.65988178
H	14.03556364	-2.68181851	1.78788843

**g. Final**

C	2.21121063	1.16000951	-0.28462257
C	4.33061755	-0.05239034	-0.08070634
C	6.46514431	-1.29153259	-0.06528589
C	8.59778773	-2.52809018	-0.15124055
C	10.72971339	-3.76319130	-0.30589500

C	4.34150606	2.38734504	0.11763799
C	6.46093453	1.17848370	-0.08312013
C	10.01530490	-0.05838182	-0.07597484
C	10.73007755	-1.29607903	-0.10436852
C	12.86237734	-2.53450331	-0.32021389
C	6.47252974	3.61964993	-0.28444462
C	8.59175529	2.40802287	-0.08104942
C	10.72774894	1.17262497	-0.07123486
C	12.86422117	-0.06084769	-0.21022322
C	14.99786527	-1.31213669	-0.41100363
C	8.60312206	4.84762761	0.11642836
C	10.72355274	3.64003187	-0.08417258
C	12.85877298	2.40277701	-0.09736073
C	14.99523099	1.15549404	-0.13531612
C	17.12999982	-0.08392595	-0.38612388
C	3.60887070	1.19634736	-0.08419872
C	5.75044457	-0.05141366	-0.05136779
C	7.88544000	-1.29050097	-0.09032167
C	10.01478700	-2.52206515	-0.17018355
C	12.13162464	-3.73213446	-0.16293086
C	5.73971292	2.42797077	-0.08556216
C	7.87975251	1.18045071	-0.10352093
C	12.14861052	-1.28818121	-0.20237121
C	14.23667123	-2.48162418	-0.64461888
C	7.87003435	3.65651238	-0.08473324
C	10.01209729	2.41122028	-0.05339362
C	12.14948790	1.17303530	-0.11284429
C	14.28345340	-0.06696534	-0.24518624
C	16.40473726	-1.29312098	-0.32874937
C	10.00158244	4.88919804	-0.08605063
C	12.14271787	3.64088870	-0.10488391
C	14.27958428	2.39611079	-0.08291319
C	16.41326141	1.15903179	-0.20365118

C	18.52026535	-0.00589715	-0.62724171
I	17.40026122	-3.01933319	0.47843041
I	14.93454423	-3.89871481	-2.09320812
I	13.09025655	-5.36685043	0.83430520
I	7.71844609	6.38048014	1.32279427
I	5.58455449	5.15810143	-1.48031561
I	3.45790360	3.91865890	1.32620729
I	1.32435278	2.69964443	-1.47949864
I	19.40219781	-1.31279633	-2.08078140
C	8.59437416	-0.05797843	-0.08671857
O	15.94536561	-0.83499437	2.42355936
O	17.15273593	-0.46709316	3.19160438
H	17.57843455	-1.34469486	3.24385128
H	15.24342863	-0.85809328	3.11064828
O	13.49424140	-1.71319343	3.20303944
H	12.61870708	-1.74775401	3.61272505
H	13.41466877	-2.23919970	2.38935491

## 8) OO Dissociation

### a. Initial

C	2.14033426	1.23328760	-0.11157123
C	4.26225598	0.01547353	-0.03280560
C	6.39116386	-1.21244814	-0.08917522
C	8.51881698	-2.43879815	-0.12815131
C	10.64311755	-3.68846991	-0.08128368
C	4.28026942	2.44717226	0.27797781
C	6.39140110	1.25138276	-0.03637605
C	9.94482276	0.01710524	-0.10224824
C	10.65639941	-1.21995059	-0.09183068
C	12.74796149	-2.48387520	0.13508924
C	6.40177308	3.69616357	-0.11349573
C	8.52763565	2.47867007	-0.04305517
C	10.66018239	1.24020212	-0.09243477
C	12.79586473	-0.00790328	-0.12105782
C	14.95928007	-1.20545223	0.13262389
C	8.54429192	4.90563997	0.27663891
C	10.65543070	3.70713145	-0.03993596
C	12.78784767	2.46884345	-0.10744904
C	14.91624106	1.24027051	-0.08917767
C	17.05852660	0.01808636	-0.08126355

C	3.54360709	1.26273307	0.05006196
C	5.68049921	0.02248768	-0.04183478
C	7.80859667	-1.20654191	-0.11736456
C	9.93579473	-2.44352292	-0.09442159
C	12.02172666	-3.65496078	0.25723027
C	5.67197013	2.49636444	0.04523140
C	7.81131720	1.25326412	-0.09108063
C	12.07453696	-1.23957231	-0.08352917
C	14.21939423	-2.47645753	0.36311964
C	7.80760085	3.72428481	0.04318021
C	9.94741765	2.47727133	-0.05129529
C	12.08401036	1.22963072	-0.11535709
C	14.22180619	0.00163181	-0.08412330
C	16.33709997	-1.15834801	0.25669695
C	9.93629583	4.95197260	0.04418542
C	12.07461070	3.70646112	-0.08925839
C	14.20405849	2.47680072	-0.09877803
C	16.33585020	1.25338781	-0.09065086
C	18.44254409	0.05229015	-0.32324782
I	17.44356197	-2.61349230	1.38853003
I	15.08340140	-3.96813193	-1.15359061
I	12.73597181	-5.34167940	1.38388922
I	7.69605531	6.37832639	1.58275646
I	5.48404323	5.29042392	-1.21363857
I	3.42753025	3.92264840	1.57816472
I	1.22197355	2.82301962	-1.21763944
I	19.30588248	-1.44656411	-1.58547217
C	8.52373469	0.01870489	-0.11024483
O	14.44346847	-2.85349734	1.82846963
O	13.83946574	-1.85173592	2.50427277

**b. Transition State 1**

C	2.14569731	1.19977648	-0.17838280
C	4.26396400	-0.01516770	-0.05756281
C	6.39232133	-1.24361568	-0.08806975
C	8.52157953	-2.46851011	-0.12417008
C	10.64640230	-3.71671922	-0.12293790
C	4.28026893	2.41638059	0.23126168
C	6.39311701	1.22079366	-0.05174941
C	9.94695924	-0.01469061	-0.09747107
C	10.65874833	-1.25194177	-0.09244800
C	12.75192622	-2.52159740	0.06743275
C	6.40850208	3.66079306	-0.16521546
C	8.52974345	2.44720442	-0.05554339
C	10.66189462	1.20933360	-0.08903314
C	12.79920347	-0.04166730	-0.11527049
C	14.96935982	-1.24028914	0.09251945

C	8.54622496	4.87658390	0.23151401
C	10.65721808	3.67706172	-0.06350463
C	12.78994285	2.43813396	-0.10348302
C	14.92080960	1.20719625	-0.08037154
C	17.06245188	-0.01252719	-0.10282407
C	3.54651126	1.23122331	-0.00441844
C	5.68170885	-0.00905200	-0.05296793
C	7.81082048	-1.23635311	-0.11347037
C	9.93847645	-2.47343377	-0.09686270
C	12.03710115	-3.70332340	0.15096250
C	5.67427864	2.46659763	0.00521380
C	7.81270419	1.22368544	-0.09445896
C	12.07532903	-1.27160435	-0.09562025
C	14.22993629	-2.52276676	0.25535327
C	7.81090158	3.69196057	0.00372478
C	9.94901463	2.44655401	-0.05912064
C	12.08709266	1.19666450	-0.10619334
C	14.22657806	-0.03016332	-0.08421069
C	16.35068868	-1.20504000	0.19556561
C	9.93804852	4.92379491	-0.00682435
C	12.07639986	3.67668090	-0.10079339
C	14.20713255	2.44353542	-0.09282262
C	16.33939674	1.22217104	-0.08597728
C	18.43860107	0.03315326	-0.39329952
I	17.47943508	-2.74438900	1.17628276
I	15.02670440	-3.87482575	-1.42993654
I	12.80633929	-5.45730090	1.12437313
I	7.69084451	6.36495433	1.51177277
I	5.49644522	5.25031278	-1.27632252
I	3.41470143	3.90270433	1.50773470
I	1.22785777	2.78274940	-1.29569728
I	19.23351599	-1.38474740	-1.78687275
C	8.52579669	-0.01028057	-0.10584261
O	14.48145947	-2.99513130	1.66318906
O	13.79495014	-2.06319321	2.37343571

**c. Transition State 2**

C	2.15746233	1.19782758	-0.22297134
C	4.27062344	-0.01682298	-0.05747516
C	6.39659544	-1.24444322	-0.08642583
C	8.52289469	-2.46988960	-0.12231967
C	10.64642719	-3.71440546	-0.11197092
C	4.28461459	2.41637653	0.21709939
C	6.39761078	1.22129187	-0.05143018
C	9.94797473	-0.01206904	-0.09342701
C	10.65614817	-1.24988992	-0.08255443
C	12.74169858	-2.51851230	0.09205885

C	6.41131569	3.65961315	-0.19327428
C	8.53348196	2.44943855	-0.06388680
C	10.66554715	1.21053447	-0.08649444
C	12.80064131	-0.04407053	-0.09801062
C	14.96962064	-1.24604856	0.08696414
C	8.55202187	4.88312812	0.17826582
C	10.66328793	3.67676674	-0.07525497
C	12.79484047	2.43669339	-0.10016888
C	14.92445855	1.20395084	-0.07440684
C	17.06347371	-0.01801494	-0.12493939
C	3.55395538	1.22980507	-0.01714790
C	5.68759771	-0.00935623	-0.05003129
C	7.81440167	-1.23731496	-0.11197887
C	9.93842501	-2.47220311	-0.08878150
C	12.03165490	-3.70796900	0.16814177
C	5.67884171	2.46684125	-0.00335000
C	7.81660067	1.22514289	-0.09484298
C	12.07066260	-1.27097530	-0.07980326
C	14.22081441	-2.52200589	0.24166353
C	7.81491510	3.69553667	-0.02436446
C	9.95341775	2.44828671	-0.06399156
C	12.09090504	1.19550801	-0.09885778
C	14.22811486	-0.03312448	-0.07002383
C	16.35534016	-1.22062875	0.14018480
C	9.94517622	4.92453247	-0.04369570
C	12.08256197	3.67534663	-0.10260334
C	14.21214121	2.44202099	-0.08901425
C	16.34179072	1.21856488	-0.08603429
C	18.43936370	0.04042005	-0.42067223
I	17.49584711	-2.84171152	0.95913175
I	14.89329850	-3.78851748	-1.58661749
I	12.80223772	-5.51066369	1.04571736
I	7.68176639	6.42423535	1.38468556
I	5.49841079	5.20485591	-1.36594152
I	3.39522866	3.92422352	1.44677676
I	1.28465282	2.74995691	-1.41461648
I	19.21411507	-1.27212347	-1.92685808
C	8.52797269	-0.00929773	-0.10431961
O	14.48394647	-3.05268284	1.61457802
O	13.58789995	-2.34643344	2.35760428

**d. Transition State 3**

C	2.15859469	1.19650100	-0.22326605
C	4.27244966	-0.01862261	-0.05750022
C	6.39908024	-1.24772998	-0.08673928
C	8.53038124	-2.47138124	-0.12933700
C	10.66112797	-3.71476438	-0.09792273



C	4.28568335	2.41469726	0.21668338
C	6.39945191	1.21965028	-0.05190863
C	9.95037622	-0.01433754	-0.09550094
C	10.65834018	-1.25080142	-0.06851475
C	12.74559932	-2.50700284	0.22758511
C	6.41193051	3.65798008	-0.19717011
C	8.53498835	2.44809371	-0.06534966
C	10.66874180	1.20934359	-0.08756383
C	12.80289840	-0.04944415	-0.08108195
C	14.98034110	-1.24847109	0.09121456
C	8.55271413	4.88179918	0.17598030
C	10.66507227	3.67503807	-0.07563629
C	12.79829121	2.43440511	-0.10336543
C	14.93007063	1.19982151	-0.07533783
C	17.06948403	-0.01937096	-0.12437325
C	3.55490621	1.22795587	-0.01743718
C	5.68963086	-0.01230803	-0.05019461
C	7.81863905	-1.23979698	-0.11369577
C	9.94268693	-2.47276567	-0.08892199
C	12.02736066	-3.71765972	0.22240254
C	5.68009965	2.46508413	-0.00481694
C	7.81798356	1.22349129	-0.09672004
C	12.07145982	-1.27121239	-0.03190312
C	14.24163634	-2.53373638	0.25023959
C	7.81578146	3.69377656	-0.02752935
C	9.95529061	2.44677628	-0.06447942
C	12.09391262	1.19306301	-0.09968471
C	14.23528361	-0.03977977	-0.06119034
C	16.36672576	-1.22201615	0.13962018
C	9.94626634	4.92274501	-0.04444022
C	12.08509129	3.67329214	-0.10363993
C	14.21558795	2.43862857	-0.09028344
C	16.34632560	1.21407502	-0.09134815
C	18.44999656	0.03868313	-0.42626366
I	17.50682677	-2.86291524	0.91024509
I	14.80862609	-3.74297897	-1.66530511
I	12.78249731	-5.55509792	1.03235677
I	7.68070513	6.42481956	1.37743887
I	5.49707607	5.20082503	-1.37040143
I	3.39635337	3.92239502	1.44618821
I	1.28812963	2.74871560	-1.41763112
I	19.19269742	-1.22539029	-1.98497305
C	8.52975322	-0.01067910	-0.10741888
O	14.52210825	-3.15027791	1.50264832
O	13.45602308	-2.43437334	2.18647156

**e. Transition State 4**

C	2.15903917	1.19626369	-0.22290519
C	4.27311037	-0.01909020	-0.05784175
C	6.40074248	-1.24873811	-0.08642962
C	8.53939242	-2.47092686	-0.13236677
C	10.67696006	-3.71614108	-0.10129684
C	4.28563754	2.41434476	0.21674844
C	6.40040058	1.21941620	-0.05221975
C	9.95219157	-0.01465385	-0.09814706
C	10.66461396	-1.24946790	-0.05579366
C	12.77447645	-2.49529173	0.40094892
C	6.41168804	3.65775047	-0.19658388
C	8.53544353	2.44794355	-0.06513270
C	10.66993370	1.20950378	-0.08807451
C	12.80042339	-0.05149388	-0.06730377
C	14.98626518	-1.24686942	0.08552012
C	8.55339076	4.88204729	0.17639794
C	10.66533118	3.67482494	-0.07587817
C	12.79993060	2.43491451	-0.10633198
C	14.93262281	1.19798127	-0.07609485
C	17.07102381	-0.01896030	-0.12247405
C	3.55527533	1.22787437	-0.01706222
C	5.69071886	-0.01277241	-0.05036257
C	7.82171363	-1.23928663	-0.11260666
C	9.94596989	-2.47068877	-0.09279350
C	12.02077757	-3.73577064	0.25172819
C	5.68072246	2.46543430	-0.00454730
C	7.81810556	1.22349809	-0.09781591
C	12.07339490	-1.25989417	0.03032254
C	14.27400311	-2.54642105	0.23248180
C	7.81570015	3.69407876	-0.02696020
C	9.95508200	2.44788363	-0.06395636
C	12.09345172	1.19429550	-0.10345288
C	14.24027071	-0.04234088	-0.05487690
C	16.37330256	-1.21747534	0.13971310
C	9.94607406	4.92309068	-0.04434788
C	12.08586814	3.67340792	-0.10405771
C	14.21671380	2.43826934	-0.09083656
C	16.34863868	1.21145833	-0.09717199
C	18.45697768	0.03490413	-0.43047841
I	17.50791231	-2.86581516	0.90589969
I	14.78870868	-3.73977740	-1.66239227
I	12.77736929	-5.56887838	1.04060194
I	7.68072862	6.42494246	1.37758295
I	5.49837052	5.20219500	-1.36778311
I	3.39681029	3.92249427	1.44634234
I	1.29001147	2.74729816	-1.41949575

I	19.18702704	-1.21959189	-1.99915369
C	8.53074845	-0.01171440	-0.10968351
O	14.55716908	-3.14873057	1.48595496
O	13.31436424	-2.46800515	2.03819426

**f. Transition State 5**

C	2.15955887	1.19656764	-0.22207865
C	4.27494496	-0.01860745	-0.05842139
C	6.40479435	-1.24890351	-0.08672245
C	8.54764119	-2.46948902	-0.13044318
C	10.68939605	-3.71986385	-0.11386345
C	4.28674057	2.41470917	0.21725083
C	6.40193939	1.21928931	-0.05242378
C	9.95801127	-0.01397624	-0.09628817
C	10.67702934	-1.24723491	-0.03975156
C	12.80550105	-2.48402484	0.52801953
C	6.41319589	3.65781954	-0.19568525
C	8.53687554	2.44896054	-0.06431431
C	10.67326071	1.21151658	-0.08764435
C	12.80606672	-0.04720676	-0.05290261
C	14.99581531	-1.25000608	0.07785770
C	8.55362658	4.88318405	0.17910133
C	10.66655892	3.67583912	-0.07468492
C	12.80191330	2.43617447	-0.10847259
C	14.93949590	1.19814177	-0.08073961
C	17.08224138	-0.01802313	-0.12225752
C	3.55637643	1.22817610	-0.01714054
C	5.69275249	-0.01259933	-0.05145872
C	7.82615260	-1.23843002	-0.11259716
C	9.95765317	-2.46997017	-0.08914404
C	12.03075601	-3.74274384	0.26898130
C	5.68153635	2.46540690	-0.00466518
C	7.82055403	1.22421535	-0.09845972
C	12.08441401	-1.25082206	0.07040863
C	14.30588558	-2.55501054	0.29372406
C	7.81695005	3.69508908	-0.02501339
C	9.95675225	2.44921774	-0.06385286
C	12.09536328	1.19834461	-0.10250148
C	14.24554686	-0.04284794	-0.05567697
C	16.37682335	-1.21330178	0.13000399
C	9.94638645	4.92399880	-0.04230539
C	12.08693827	3.67457918	-0.10507018
C	14.22091778	2.43815809	-0.09288230
C	16.35746562	1.21640425	-0.09561066
C	18.46045185	0.03237434	-0.43676634
I	17.49679899	-2.86324243	0.90334468
I	14.75356603	-3.74167667	-1.70568229

I	12.78348283	-5.55763443	1.06441350
I	7.67962745	6.42696925	1.37687040
I	5.49758852	5.20113553	-1.36982510
I	3.39776276	3.92239215	1.44614789
I	1.28979268	2.74815056	-1.41803642
I	19.18965353	-1.21979556	-2.00275394
C	8.53547634	-0.01090550	-0.11105063
O	14.70437563	-3.16622702	1.43556935
O	13.02075305	-2.40120675	1.98764427

**g. Final**

C	2.15262115	1.19911660	-0.17778652
C	4.27383930	-0.01349225	-0.05897160
C	6.40667500	-1.24540781	-0.10060534
C	8.54541881	-2.47466162	-0.19242870
C	10.66553593	-3.72953976	-0.34836967
C	4.28818991	2.41731099	0.22968612
C	6.40257539	1.21954915	-0.05863277
C	9.95965529	-0.01935144	-0.07203417
C	10.67854768	-1.25263240	-0.00251482
C	12.79051361	-2.45787731	0.43650476
C	6.41378366	3.65925198	-0.17792228
C	8.53657940	2.44727942	-0.06154684
C	10.67133690	1.21115014	-0.07754900
C	12.80679374	-0.02066372	-0.02055832
C	15.00844694	-1.23535405	0.08689935
C	8.55043606	4.87681149	0.22654005
C	10.66381442	3.67819885	-0.06436158
C	12.80154430	2.44658671	-0.10805738
C	14.93661121	1.20443153	-0.14823317
C	17.06512121	-0.01172269	-0.44864216
C	3.55376326	1.23202149	-0.00252824
C	5.69316477	-0.01033472	-0.05819629
C	7.82816641	-1.24196983	-0.12453701
C	9.96149062	-2.49715642	-0.11427230
C	12.07569068	-3.74987343	0.15532872
C	5.68134174	2.46576995	-0.00271187
C	7.82157427	1.22133265	-0.09922349
C	12.08291229	-1.21960405	0.09699987
C	14.28950260	-2.39192067	0.67877637
C	7.81644036	3.69202849	-0.00606546
C	9.95521119	2.44935464	-0.06105600
C	12.09282424	1.21322898	-0.08884741
C	14.24713357	-0.02685251	-0.05959124
C	16.38770769	-1.23070057	-0.14294840
C	9.94281907	4.92469142	-0.00663827
C	12.08441900	3.68160305	-0.10250725

C	14.22021835	2.44448861	-0.11597811
C	16.35547745	1.21415525	-0.25651810
C	18.45327884	0.09339428	-0.80316723
I	17.55637124	-2.98647315	0.20107823
I	14.37537448	-3.65231050	-2.66176403
I	13.34394457	-5.55580831	-0.11361381
I	7.69103877	6.36390972	1.50490051
I	5.50009712	5.24160871	-1.29625887
I	3.42991660	3.90358825	1.51006556
I	1.24148097	2.78235935	-1.29684504
I	19.12462713	-1.03548564	-2.48837127
C	8.53640836	-0.01411022	-0.10357201
O	14.79507994	-3.19832566	1.45071977
O	12.11553802	-3.25762937	1.46995723

## Mulliken Charges

### 1. Chlorine

#### a. Bare

#### POPULATION ANALYSIS

-----					
	iatm	typnm	znuc	rho(u)	rho(d) popul
-----					
1	C	4.00000	2.01778	2.01778	-0.03556
2	C	4.00000	2.01450	2.01450	-0.02900
3	C	4.00000	1.98136	1.98136	0.03728
4	C	4.00000	1.97864	1.97864	0.04271
5	C	4.00000	2.03269	2.03269	-0.06538
6	C	4.00000	2.02256	2.02256	-0.04512
7	C	4.00000	1.98318	1.98318	0.03364
8	C	4.00000	1.97523	1.97523	0.04954
9	C	4.00000	1.99350	1.99350	0.01300
10	C	4.00000	2.01758	2.01758	-0.03516
11	C	4.00000	2.01518	2.01518	-0.03036
12	C	4.00000	2.01904	2.01904	-0.03808

13	C	4.00000	1.98328	1.98328	0.03345
14	C	4.00000	1.97971	1.97971	0.04059
15	C	4.00000	2.03838	2.03838	-0.07676
16	C	4.00000	2.02107	2.02107	-0.04214
17	C	4.00000	1.98560	1.98560	0.02880
18	C	4.00000	1.91235	1.91235	0.17530
19	C	4.00000	1.98926	1.98926	0.02148
20	C	4.00000	2.02217	2.02217	-0.04435
21	C	4.00000	1.99615	1.99615	0.00770
22	C	4.00000	1.97734	1.97734	0.04532
23	C	4.00000	1.98308	1.98308	0.03385
24	C	4.00000	1.97034	1.97034	0.05933
25	C	4.00000	2.01759	2.01759	-0.03517
26	C	4.00000	1.98994	1.98994	0.02012
27	C	4.00000	2.00656	2.00656	-0.01312
28	C	4.00000	1.95309	1.95309	0.09383
29	C	4.00000	2.01416	2.01416	-0.02831
30	C	4.00000	2.00118	2.00118	-0.00235
31	C	4.00000	1.97559	1.97559	0.04883
32	C	4.00000	1.98730	1.98730	0.02541
33	C	4.00000	1.97011	1.97011	0.05978
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>2.01374</b>	<b>2.01374</b>	<b>-0.02748</b>
35	C	4.00000	1.98866	1.98866	0.02269
36	C	4.00000	2.00901	2.00901	-0.01802
37	C	4.00000	1.98289	1.98289	0.03421
38	C	4.00000	1.94693	1.94693	0.10615
39	C	4.00000	2.01296	2.01296	-0.02591
40	Cl	7.00000	3.53731	3.53731	-0.07461
41	Cl	7.00000	3.53715	3.53715	-0.07431
42	Cl	7.00000	3.53730	3.53730	-0.07460
43	Cl	7.00000	3.53675	3.53675	-0.07350
44	Cl	7.00000	3.53759	3.53759	-0.07518
45	Cl	7.00000	3.53749	3.53749	-0.07498

46	Cl	7.00000	3.53821	3.53821	-0.07641
47	Cl	7.00000	3.53720	3.53720	-0.07441
48	C	4.00000	1.92135	1.92135	0.15730
-----					
total charge	216.00000	108.00000	108.00000	0.00000	
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**b. OOH**

-----					
iatm typnm		znuc	rho(u)	rho(d)	popul
-----					
1	C	4.00000	2.16227	1.86380	-0.02608
2	C	4.00000	2.06545	1.96513	-0.03058
3	C	4.00000	1.99410	1.95932	0.04659
4	C	4.00000	1.98562	1.96924	0.04514
5	C	4.00000	2.02962	2.01736	-0.04698
6	C	4.00000	2.16970	1.87663	-0.04633
7	C	4.00000	2.01953	1.92139	0.05908
8	C	4.00000	1.95600	1.98876	0.05524
9	C	4.00000	1.98410	1.96831	0.04759
10	C	4.00000	2.02003	2.00772	-0.02775
11	C	4.00000	2.16141	1.86393	-0.02534
12	C	4.00000	2.06365	1.96571	-0.02936
13	C	4.00000	2.00408	1.96863	0.02729
14	C	4.00000	1.99921	1.98325	0.01754
15	C	4.00000	2.01588	2.00258	-0.01846
16	C	4.00000	2.17018	1.87328	-0.04346
17	C	4.00000	2.01782	1.92034	0.06184
18	C	4.00000	1.92061	1.88552	0.19387
19	C	4.00000	1.95553	1.93518	0.10928
20	C	4.00000	1.99097	1.97821	0.03083
21	C	4.00000	1.94329	2.06212	-0.00542
22	C	4.00000	1.94586	2.00564	0.04850
23	C	4.00000	1.96103	1.98970	0.04927

24	C	4.00000	1.97281	1.98685	0.04034
25	C	4.00000	2.00856	2.04039	-0.04895
26	C	4.00000	1.92663	2.04552	0.02785
27	C	4.00000	1.98812	2.04536	-0.03348
28	C	4.00000	1.95223	1.96575	0.08201
29	C	4.00000	2.01742	2.03911	-0.05653
30	C	4.00000	1.94247	2.06242	-0.00489
31	C	4.00000	1.95141	2.00916	0.03943
32	C	4.00000	1.96368	1.99257	0.04375
33	C	4.00000	1.99117	2.01548	-0.00665
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>1.92626</b>	<b>1.92734</b>	<b>0.14640</b>
35	C	4.00000	1.92716	2.04678	0.02606
36	C	4.00000	1.98871	2.04749	-0.03620
37	C	4.00000	1.96084	1.98537	0.05378
38	C	4.00000	1.98042	2.00550	0.01408
39	C	4.00000	2.01673	2.03654	-0.05327
40	Cl	7.00000	3.55489	3.55494	-0.10983
41	Cl	7.00000	3.53362	3.53668	-0.07029
42	Cl	7.00000	3.53735	3.54182	-0.07917
43	Cl	7.00000	3.55608	3.51915	-0.07523
44	Cl	7.00000	3.55632	3.51980	-0.07612
45	Cl	7.00000	3.55604	3.51963	-0.07566
46	Cl	7.00000	3.55628	3.51957	-0.07585
47	Cl	7.00000	3.53640	3.53914	-0.07554
48	C	4.00000	1.93950	1.90383	0.15667
49	O	6.00000	3.13461	3.13394	-0.26855
50	O	6.00000	3.19249	3.19223	-0.38472
51	H	1.00000	0.29587	0.29588	0.40825

-----  
total charge 229.00000 115.00000 114.00000 0.00000  
-----

c. O



-----					
iatm typnm		znuc	rho(u)	rho(d)	popul
-----					
1	C	4.00000	2.01620	2.01620	-0.03240
2	C	4.00000	2.00441	2.00441	-0.00882
3	C	4.00000	1.98279	1.98279	0.03443
4	C	4.00000	1.97360	1.97360	0.05281
5	C	4.00000	2.03389	2.03389	-0.06778
6	C	4.00000	2.02343	2.02343	-0.04686
7	C	4.00000	1.98356	1.98356	0.03288
8	C	4.00000	1.98184	1.98184	0.03631
9	C	4.00000	1.97284	1.97284	0.05432
10	C	4.00000	2.01538	2.01538	-0.03076
11	C	4.00000	2.01779	2.01779	-0.03558
12	C	4.00000	2.01607	2.01607	-0.03215
13	C	4.00000	1.98489	1.98489	0.03021
14	C	4.00000	2.01186	2.01186	-0.02373
15	C	4.00000	2.03760	2.03760	-0.07520
16	C	4.00000	2.02080	2.02080	-0.04161
17	C	4.00000	1.96881	1.96881	0.06238
18	C	4.00000	1.92546	1.92546	0.14908
19	C	4.00000	2.03509	2.03509	-0.07018
20	C	4.00000	2.01559	2.01559	-0.03119
21	C	4.00000	1.99900	1.99900	0.00200
22	C	4.00000	1.97678	1.97678	0.04644
23	C	4.00000	1.95773	1.95773	0.08455
24	C	4.00000	1.98061	1.98061	0.03879
25	C	4.00000	2.01044	2.01044	-0.02087
26	C	4.00000	1.98843	1.98843	0.02313
27	C	4.00000	1.98003	1.98003	0.03995
28	C	4.00000	1.93601	1.93601	0.12798
29	C	4.00000	1.98896	1.98896	0.02209
30	C	4.00000	1.99848	1.99848	0.00305

31	C	4.00000	1.97506	1.97506	0.04989
32	C	4.00000	1.99010	1.99010	0.01980
33	C	4.00000	1.93392	1.93392	0.13217
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>1.86526</b>	<b>1.86526</b>	<b>0.26947</b>
35	C	4.00000	1.98899	1.98899	0.02203
36	C	4.00000	2.01183	2.01183	-0.02366
37	C	4.00000	1.96013	1.96013	0.07974
38	C	4.00000	1.95748	1.95748	0.08503
39	C	4.00000	2.01034	2.01034	-0.02067
40	Cl	7.00000	3.55069	3.55069	-0.10137
41	Cl	7.00000	3.53253	3.53253	-0.06506
42	Cl	7.00000	3.53345	3.53345	-0.06690
43	Cl	7.00000	3.53600	3.53600	-0.07200
44	Cl	7.00000	3.53673	3.53673	-0.07347
45	Cl	7.00000	3.53617	3.53617	-0.07234
46	Cl	7.00000	3.53642	3.53642	-0.07284
47	Cl	7.00000	3.53263	3.53263	-0.06526
48	C	4.00000	1.95072	1.95072	0.09857
49	O	6.00000	3.22320	3.22320	-0.44639

-----  
total charge 222.00000 111.00000 111.00000 0.00000  
-----

**d. OH**

	iatm	typnm	znuc	rho(u)	rho(d)	popul
-----						
1	C	4.00000	2.16027	1.86746	-0.02773	
2	C	4.00000	2.06027	1.96507	-0.02534	
3	C	4.00000	2.00270	1.97052	0.02677	
4	C	4.00000	1.97938	1.96571	0.05490	
5	C	4.00000	2.02639	2.01627	-0.04266	
6	C	4.00000	2.16571	1.87742	-0.04313	

7	C	4.00000	2.01739	1.92354	0.05907
8	C	4.00000	1.94217	1.97219	0.08564
9	C	4.00000	1.99435	1.98049	0.02516
10	C	4.00000	2.01757	2.00721	-0.02478
11	C	4.00000	2.16071	1.86743	-0.02814
12	C	4.00000	2.06683	1.97410	-0.04093
13	C	4.00000	2.01656	1.98381	-0.00037
14	C	4.00000	1.99434	1.98064	0.02502
15	C	4.00000	2.01158	2.00047	-0.01205
16	C	4.00000	2.16700	1.87553	-0.04253
17	C	4.00000	2.02046	1.92714	0.05241
18	C	4.00000	1.93609	1.90444	0.15947
19	C	4.00000	1.97522	1.95771	0.06707
20	C	4.00000	2.01113	2.00051	-0.01164
21	C	4.00000	1.94623	2.05902	-0.00524
22	C	4.00000	1.94684	2.00293	0.05023
23	C	4.00000	1.96439	1.99039	0.04522
24	C	4.00000	1.98002	1.99221	0.02777
25	C	4.00000	2.00986	2.03824	-0.04810
26	C	4.00000	1.93343	2.04648	0.02009
27	C	4.00000	1.97239	2.02581	0.00181
28	C	4.00000	1.94820	1.96001	0.09179
29	C	4.00000	2.01789	2.03580	-0.05369
30	C	4.00000	1.94492	2.05918	-0.00410
31	C	4.00000	1.94246	1.99667	0.06086
32	C	4.00000	1.95837	1.98457	0.05707
33	C	4.00000	1.99241	2.01454	-0.00694
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>1.92913</b>	<b>1.92997</b>	<b>0.14090</b>
35	C	4.00000	1.93181	2.04507	0.02312
36	C	4.00000	1.97915	2.03444	-0.01359
37	C	4.00000	1.95314	1.97537	0.07149
38	C	4.00000	1.97398	1.99645	0.02957
39	C	4.00000	2.02059	2.03743	-0.05802

40	Cl	7.00000	3.55403	3.55409	-0.10813
41	Cl	7.00000	3.53561	3.53830	-0.07390
42	Cl	7.00000	3.53904	3.54315	-0.08220
43	Cl	7.00000	3.55626	3.51955	-0.07580
44	Cl	7.00000	3.55655	3.51933	-0.07588
45	Cl	7.00000	3.55604	3.51972	-0.07575
46	Cl	7.00000	3.55661	3.51941	-0.07602
47	Cl	7.00000	3.53502	3.53749	-0.07250
48	C	4.00000	1.95633	1.92401	0.11966
49	O	6.00000	3.28780	3.28740	-0.57520
50	H	1.00000	0.29538	0.29533	0.40929

-----  
total charge 223.00000 112.00000 111.00000 0.00000  
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**e. HOH formation Transition State**

	iatm	typnm	znuc	rho(u)	rho(d)	popul
-----						
1	C	4.00000	2.01659	2.01659	-0.03319	
2	C	4.00000	2.03093	2.03093	-0.06186	
3	C	4.00000	2.01887	2.01887	-0.03773	
4	C	4.00000	2.00514	2.00514	-0.01028	
5	C	4.00000	2.02685	2.02685	-0.05370	
6	C	4.00000	2.02482	2.02482	-0.04963	
7	C	4.00000	1.92831	1.92831	0.14338	
8	C	4.00000	1.98378	1.98378	0.03245	
9	C	4.00000	1.96292	1.96292	0.07415	
10	C	4.00000	1.99738	1.99738	0.00524	
11	C	4.00000	2.00710	2.00710	-0.01419	
12	C	4.00000	2.00545	2.00545	-0.01090	
13	C	4.00000	1.99622	1.99622	0.00756	
14	C	4.00000	2.02457	2.02457	-0.04915	

15	C	4.00000	2.05026	2.05026	-0.10052
16	C	4.00000	2.02700	2.02700	-0.05400
17	C	4.00000	1.98726	1.98726	0.02547
18	C	4.00000	1.96193	1.96193	0.07615
19	C	4.00000	2.01511	2.01511	-0.03022
20	C	4.00000	2.00669	2.00669	-0.01339
21	C	4.00000	2.00032	2.00032	-0.00063
22	C	4.00000	2.00521	2.00521	-0.01042
23	C	4.00000	2.02676	2.02676	-0.05353
24	C	4.00000	2.00510	2.00510	-0.01020
25	C	4.00000	1.98942	1.98942	0.02117
26	C	4.00000	2.00132	2.00132	-0.00264
27	C	4.00000	2.01512	2.01512	-0.03025
28	C	4.00000	1.91274	1.91274	0.17453
29	C	4.00000	2.14821	2.14821	-0.29643
30	C	4.00000	1.99964	1.99964	0.00071
31	C	4.00000	1.96169	1.96169	0.07662
32	C	4.00000	1.97772	1.97772	0.04456
33	C	4.00000	1.93921	1.93921	0.12158
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>1.92742</b>	<b>1.92742</b>	<b>0.14515</b>
35	C	4.00000	1.98034	1.98034	0.03933
36	C	4.00000	1.94286	1.94286	0.11429
37	C	4.00000	1.88015	1.88015	0.23971
38	C	4.00000	1.95439	1.95439	0.09121
39	C	4.00000	2.02378	2.02378	-0.04757
40	Cl	7.00000	3.55297	3.55297	-0.10595
41	Cl	7.00000	3.58429	3.58429	-0.16858
42	Cl	7.00000	3.54334	3.54334	-0.08669
43	Cl	7.00000	3.53720	3.53720	-0.07440
44	Cl	7.00000	3.53673	3.53673	-0.07345
45	Cl	7.00000	3.53840	3.53840	-0.07679
46	Cl	7.00000	3.53515	3.53515	-0.07031
47	Cl	7.00000	3.52574	3.52574	-0.05149

48	C	4.00000	1.90297	1.90297	0.19406
49	O	6.00000	3.32463	3.32463	-0.64925
50	H	1.00000	0.29055	0.29055	0.41890
51	H	1.00000	0.28100	0.28100	0.43799
52	O	6.00000	3.40983	3.40983	-0.81967
53	H	1.00000	0.30136	0.30136	0.39728
54	H	1.00000	0.36725	0.36725	0.26550
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total charge		232.00000	116.00000	116.00000	0.00000
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## 2. Bromine

### a. Bare

-----					
iatm typnm		znuc	rho(u)	rho(d)	popul
-----					
1	C	4.00000	2.16401	2.16401	-0.32801
2	C	4.00000	2.01706	2.01706	-0.03412
3	C	4.00000	1.98039	1.98039	0.03922
4	C	4.00000	1.97763	1.97763	0.04474
5	C	4.00000	1.96018	1.96018	0.07964
6	C	4.00000	2.16913	2.16913	-0.33826
7	C	4.00000	1.98812	1.98812	0.02376
8	C	4.00000	1.98022	1.98022	0.03955
9	C	4.00000	1.99667	1.99667	0.00667
10	C	4.00000	1.94632	1.94632	0.10735
11	C	4.00000	2.16262	2.16262	-0.32524
12	C	4.00000	2.02228	2.02228	-0.04456
13	C	4.00000	1.98322	1.98322	0.03357
14	C	4.00000	1.97965	1.97965	0.04071
15	C	4.00000	1.96584	1.96584	0.06833
16	C	4.00000	2.16842	2.16842	-0.33684
17	C	4.00000	1.98933	1.98933	0.02134

18	C	4.00000	1.91941	1.91941	0.16117
19	C	4.00000	1.99473	1.99473	0.01053
20	C	4.00000	1.95102	1.95102	0.09797
21	C	4.00000	1.92675	1.92675	0.14650
22	C	4.00000	1.97889	1.97889	0.04222
23	C	4.00000	1.97375	1.97375	0.05249
24	C	4.00000	1.97520	1.97520	0.04960
25	C	4.00000	2.16567	2.16567	-0.33135
26	C	4.00000	1.91935	1.91935	0.16129
27	C	4.00000	2.00568	2.00568	-0.01136
28	C	4.00000	1.95787	1.95787	0.08426
29	C	4.00000	2.16127	2.16127	-0.32254
30	C	4.00000	1.92955	1.92955	0.14091
31	C	4.00000	1.97646	1.97646	0.04708
32	C	4.00000	1.97629	1.97629	0.04743
33	C	4.00000	1.97408	1.97408	0.05183
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>2.16159</b>	<b>2.16159</b>	<b>-0.32318</b>
35	C	4.00000	1.91810	1.91810	0.16379
36	C	4.00000	2.00779	2.00779	-0.01557
37	C	4.00000	1.98622	1.98622	0.02755
38	C	4.00000	1.95113	1.95113	0.09774
39	C	4.00000	2.16015	2.16015	-0.32030
40	Br	7.00000	3.45638	3.45638	0.08724
41	Br	7.00000	3.45603	3.45603	0.08795
42	Br	7.00000	3.45645	3.45645	0.08710
43	Br	7.00000	3.45635	3.45635	0.08730
44	Br	7.00000	3.45664	3.45664	0.08671
45	Br	7.00000	3.45654	3.45654	0.08692
46	Br	7.00000	3.45744	3.45744	0.08512
47	Br	7.00000	3.45609	3.45609	0.08783
48	C	4.00000	1.92604	1.92604	0.14792

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total charge	216.00000	108.00000	108.00000	0.00000
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**b. OOH**

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	iatm	typnm	znuc	rho(u)	rho(d)	popul
-----						
1	C	4.00000	2.31690	2.00036	-0.31726	
2	C	4.00000	2.06950	1.97048	-0.03998	
3	C	4.00000	1.99518	1.95994	0.04488	
4	C	4.00000	1.98665	1.96975	0.04360	
5	C	4.00000	1.96382	1.94999	0.08619	
6	C	4.00000	2.32588	2.01512	-0.34100	
7	C	4.00000	2.02489	1.92772	0.04739	
8	C	4.00000	1.95819	1.99144	0.05037	
9	C	4.00000	1.98527	1.96883	0.04590	
10	C	4.00000	1.95614	1.94214	0.10172	
11	C	4.00000	2.31558	2.00107	-0.31666	
12	C	4.00000	2.06547	1.96842	-0.03388	
13	C	4.00000	2.00089	1.96525	0.03386	
14	C	4.00000	2.00136	1.98489	0.01375	
15	C	4.00000	1.96880	1.95409	0.07711	
16	C	4.00000	2.32617	2.01202	-0.33819	
17	C	4.00000	2.02315	1.92640	0.05045	
18	C	4.00000	1.91906	1.88410	0.19684	
19	C	4.00000	1.95058	1.92956	0.11986	
20	C	4.00000	1.93934	1.92521	0.13545	
21	C	4.00000	1.87022	1.99584	0.13394	
22	C	4.00000	1.94543	2.00536	0.04921	
23	C	4.00000	1.95994	1.98909	0.05097	
24	C	4.00000	1.97484	1.98960	0.03556	
25	C	4.00000	2.14440	2.18125	-0.32564	
26	C	4.00000	1.85334	1.97886	0.16780	
27	C	4.00000	1.98861	2.04574	-0.03434	
28	C	4.00000	1.95352	1.96740	0.07908	



29	C	4.00000	2.15848	2.18465	-0.34313
30	C	4.00000	1.86882	1.99547	0.13570
31	C	4.00000	1.95349	2.01153	0.03498
32	C	4.00000	1.96358	1.99291	0.04351
33	C	4.00000	1.99775	2.02305	-0.02080
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>2.02796</b>	<b>2.02926</b>	<b>-0.05722</b>
35	C	4.00000	1.85376	1.98021	0.16602
36	C	4.00000	1.98762	2.04636	-0.03398
37	C	4.00000	1.96062	1.98563	0.05375
38	C	4.00000	1.98660	2.01267	0.00073
39	C	4.00000	2.16119	2.18476	-0.34595
40	Br	7.00000	3.49470	3.49475	0.01055
41	Br	7.00000	3.45241	3.45500	0.09259
42	Br	7.00000	3.45788	3.46150	0.08063
43	Br	7.00000	3.47142	3.44224	0.08634
44	Br	7.00000	3.47162	3.44293	0.08545
45	Br	7.00000	3.47107	3.44214	0.08679
46	Br	7.00000	3.47147	3.44265	0.08588
47	Br	7.00000	3.45567	3.45792	0.08641
48	C	4.00000	1.93762	1.90211	0.16027
49	O	6.00000	3.12538	3.12471	-0.25009
50	O	6.00000	3.19007	3.18987	-0.37994
51	H	1.00000	0.29772	0.29773	0.40455

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total charge 229.00000 115.00000 114.00000 0.00000  
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**c. O**

	iatm	typnm	znuc	rho(u)	rho(d)	popul
-----						
1	C	4.00000	2.16263	2.16263	-0.32526	
2	C	4.00000	2.00765	2.00765	-0.01529	
3	C	4.00000	1.97911	1.97911	0.04179	

4	C	4.00000	1.97676	1.97676	0.04649
5	C	4.00000	1.96321	1.96321	0.07359
6	C	4.00000	2.17058	2.17058	-0.34117
7	C	4.00000	1.98736	1.98736	0.02528
8	C	4.00000	1.98190	1.98190	0.03619
9	C	4.00000	1.97276	1.97276	0.05449
10	C	4.00000	1.95288	1.95288	0.09424
11	C	4.00000	2.16421	2.16421	-0.32842
12	C	4.00000	2.01824	2.01824	-0.03647
13	C	4.00000	1.98332	1.98332	0.03336
14	C	4.00000	2.01379	2.01379	-0.02757
15	C	4.00000	1.99328	1.99328	0.01345
16	C	4.00000	2.16842	2.16842	-0.33685
17	C	4.00000	1.97317	1.97317	0.05367
18	C	4.00000	1.92671	1.92671	0.14659
19	C	4.00000	2.03354	2.03354	-0.06708
20	C	4.00000	1.95406	1.95406	0.09188
21	C	4.00000	1.92896	1.92896	0.14207
22	C	4.00000	1.97766	1.97766	0.04467
23	C	4.00000	1.96029	1.96029	0.07941
24	C	4.00000	1.98571	1.98571	0.02857
25	C	4.00000	2.15407	2.15407	-0.30813
26	C	4.00000	1.91888	1.91888	0.16224
27	C	4.00000	1.98101	1.98101	0.03799
28	C	4.00000	1.93919	1.93919	0.12162
29	C	4.00000	2.12941	2.12941	-0.25882
30	C	4.00000	1.92853	1.92853	0.14294
31	C	4.00000	1.97671	1.97671	0.04658
32	C	4.00000	1.99104	1.99104	0.01791
33	C	4.00000	1.93018	1.93018	0.13964
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>1.98189</b>	<b>1.98189</b>	<b>0.03623</b>
35	C	4.00000	1.91902	1.91902	0.16196
36	C	4.00000	2.01186	2.01186	-0.02372

37	C	4.00000	1.95937	1.95937	0.08125
38	C	4.00000	1.96340	1.96340	0.07320
39	C	4.00000	2.15942	2.15942	-0.31884
40	Br	7.00000	3.48586	3.48586	0.02828
41	Br	7.00000	3.44701	3.44701	0.10598
42	Br	7.00000	3.45145	3.45145	0.09710
43	Br	7.00000	3.45481	3.45481	0.09039
44	Br	7.00000	3.45576	3.45576	0.08848
45	Br	7.00000	3.45505	3.45505	0.08991
46	Br	7.00000	3.45554	3.45554	0.08892
47	Br	7.00000	3.45155	3.45155	0.09690
48	C	4.00000	1.95188	1.95188	0.09624
49	O	6.00000	3.21092	3.21092	-0.42184

-----  
total charge 222.00000 111.00000 111.00000 0.00000  
-----

**d. OH**

		iatm	typnm	znuc	rho(u)	rho(d)	popul
-----							
		1	C	4.00000	2.31743	2.00313	-0.32057
		2	C	4.00000	2.06386	1.96474	-0.02861
		3	C	4.00000	2.00297	1.96761	0.02943
		4	C	4.00000	1.98037	1.96360	0.05603
		5	C	4.00000	1.96057	1.94715	0.09228
		6	C	4.00000	2.32577	2.01211	-0.33788
		7	C	4.00000	2.02692	1.92874	0.04434
		8	C	4.00000	1.94261	1.97667	0.08071
		9	C	4.00000	1.99613	1.97976	0.02411
		10	C	4.00000	1.95365	1.94000	0.10635
		11	C	4.00000	2.31700	2.00362	-0.32062
		12	C	4.00000	2.06923	1.97244	-0.04167

13	C	4.00000	2.01881	1.98253	-0.00134
14	C	4.00000	1.99705	1.98061	0.02234
15	C	4.00000	1.96439	1.95006	0.08555
16	C	4.00000	2.32646	2.00924	-0.33570
17	C	4.00000	2.02854	1.93127	0.04019
18	C	4.00000	1.93858	1.90378	0.15764
19	C	4.00000	1.97191	1.95090	0.07719
20	C	4.00000	1.96233	1.94864	0.08903
21	C	4.00000	1.86913	1.99524	0.13562
22	C	4.00000	1.94428	2.00533	0.05040
23	C	4.00000	1.96384	1.99309	0.04307
24	C	4.00000	1.98206	1.99670	0.02124
25	C	4.00000	2.14348	2.17947	-0.32295
26	C	4.00000	1.85849	1.98471	0.15680
27	C	4.00000	1.96018	2.01760	0.02222
28	C	4.00000	1.94948	1.96377	0.08675
29	C	4.00000	2.15883	2.18245	-0.34128
30	C	4.00000	1.86758	1.99510	0.13732
31	C	4.00000	1.94127	2.00030	0.05844
32	C	4.00000	1.95730	1.98656	0.05613
33	C	4.00000	1.99745	2.02329	-0.02074
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>2.02850</b>	<b>2.02984</b>	<b>-0.05834</b>
35	C	4.00000	1.85672	1.98335	0.15992
36	C	4.00000	1.97577	2.03501	-0.01078
37	C	4.00000	1.95029	1.97564	0.07406
38	C	4.00000	1.98116	2.00711	0.01173
39	C	4.00000	2.16248	2.18504	-0.34753
40	Br	7.00000	3.49429	3.49436	0.01135
41	Br	7.00000	3.45497	3.45732	0.08770
42	Br	7.00000	3.45924	3.46262	0.07815
43	Br	7.00000	3.47150	3.44300	0.08549
44	Br	7.00000	3.47176	3.44290	0.08534
45	Br	7.00000	3.47126	3.44296	0.08577

46	Br	7.00000	3.47176	3.44280	0.08544
47	Br	7.00000	3.45413	3.45626	0.08961
48	C	4.00000	1.96481	1.92873	0.10647
49	O	6.00000	3.27894	3.27846	-0.55739
50	H	1.00000	0.29447	0.29438	0.41115
-----					
total charge		223.00000	112.00000	111.00000	0.00000
-----					

**e. HOH formation Transition State**

-----					
iatm typnm		znuc	rho(u)	rho(d)	popul
-----					
1	C	4.00000	2.16450	2.16450	-0.32901
2	C	4.00000	2.03296	2.03296	-0.06593
3	C	4.00000	2.02056	2.02056	-0.04113
4	C	4.00000	2.00893	2.00893	-0.01787
5	C	4.00000	1.95805	1.95805	0.08391
6	C	4.00000	2.16922	2.16922	-0.33844
7	C	4.00000	1.92827	1.92827	0.14346
8	C	4.00000	1.99419	1.99419	0.01163
9	C	4.00000	1.94521	1.94521	0.10957
10	C	4.00000	1.95283	1.95283	0.09434
11	C	4.00000	2.15102	2.15102	-0.30204
12	C	4.00000	2.00955	2.00955	-0.01910
13	C	4.00000	1.99631	1.99631	0.00739
14	C	4.00000	2.01765	2.01765	-0.03530
15	C	4.00000	2.02018	2.02018	-0.04037
16	C	4.00000	2.17210	2.17210	-0.34420
17	C	4.00000	1.99637	1.99637	0.00725
18	C	4.00000	1.96397	1.96397	0.07207
19	C	4.00000	2.01040	2.01040	-0.02081
20	C	4.00000	1.96736	1.96736	0.06529

21	C	4.00000	1.92908	1.92908	0.14185
22	C	4.00000	2.01690	2.01690	-0.03379
23	C	4.00000	2.05563	2.05563	-0.11126
24	C	4.00000	2.00958	2.00958	-0.01916
25	C	4.00000	2.12993	2.12993	-0.25987
26	C	4.00000	1.93532	1.93532	0.12936
27	C	4.00000	2.01668	2.01668	-0.03336
28	C	4.00000	1.91770	1.91770	0.16461
29	C	4.00000	2.20987	2.20987	-0.41974
30	C	4.00000	1.92864	1.92864	0.14273
31	C	4.00000	1.96278	1.96278	0.07444
32	C	4.00000	1.98132	1.98132	0.03736
33	C	4.00000	1.95050	1.95050	0.09901
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>2.02509</b>	<b>2.02509</b>	<b>-0.05018</b>
35	C	4.00000	1.90651	1.90651	0.18699
36	C	4.00000	1.93476	1.93476	0.13049
37	C	4.00000	1.86972	1.86972	0.26056
38	C	4.00000	1.95477	1.95477	0.09045
39	C	4.00000	2.16487	2.16487	-0.32973
40	Br	7.00000	3.48920	3.48920	0.02160
41	Br	7.00000	3.55476	3.55476	-0.10952
42	Br	7.00000	3.46556	3.46556	0.06887
43	Br	7.00000	3.45546	3.45546	0.08909
44	Br	7.00000	3.45490	3.45490	0.09020
45	Br	7.00000	3.45768	3.45768	0.08463
46	Br	7.00000	3.45297	3.45297	0.09406
47	Br	7.00000	3.43740	3.43740	0.12520
48	C	4.00000	1.88765	1.88765	0.22471
49	O	6.00000	3.31502	3.31502	-0.63003
50	H	1.00000	0.28990	0.28990	0.42020
51	H	1.00000	0.28152	0.28152	0.43697
52	O	6.00000	3.40823	3.40823	-0.81646
53	H	1.00000	0.30135	0.30135	0.39731

54	H	1.00000	0.36914	0.36914	0.26171
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total charge	232.00000	116.00000	116.00000	0.00000
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### 3. Iodine

#### a. Bare

	iatm	typnm	znuc	rho(u)	rho(d)
	popul				
1	C	4.00000	2.22577	2.22577	-0.45155
2	C	4.00000	2.02476	2.02476	-0.04952
3	C	4.00000	1.97670	1.97670	0.04659
4	C	4.00000	1.98763	1.98763	0.02473
5	C	4.00000	1.88855	1.88855	0.22290
6	C	4.00000	2.23094	2.23094	-0.46189
7	C	4.00000	1.99575	1.99575	0.00849
8	C	4.00000	1.98126	1.98126	0.03749
9	C	4.00000	1.99592	1.99592	0.00816
10	C	4.00000	1.88666	1.88666	0.22668
11	C	4.00000	2.22602	2.22602	-0.45204
12	C	4.00000	2.02320	2.02320	-0.04641
13	C	4.00000	1.97933	1.97933	0.04133
14	C	4.00000	1.98618	1.98618	0.02763
15	C	4.00000	1.89235	1.89235	0.21531
16	C	4.00000	2.23032	2.23032	-0.46064
17	C	4.00000	2.00182	2.00182	-0.00363
18	C	4.00000	1.91928	1.91928	0.16144
19	C	4.00000	1.98746	1.98746	0.02507
20	C	4.00000	1.88271	1.88271	0.23459
21	C	4.00000	1.88702	1.88702	0.22596
22	C	4.00000	1.97877	1.97877	0.04247
23	C	4.00000	1.97245	1.97245	0.05509
24	C	4.00000	2.01191	2.01191	-0.02383

25	C	4.00000	2.22839	2.22839	-0.45678
26	C	4.00000	1.88309	1.88309	0.23383
27	C	4.00000	1.99451	1.99451	0.01098
28	C	4.00000	1.98927	1.98927	0.02146
29	C	4.00000	2.22491	2.22491	-0.44982
30	C	4.00000	1.89312	1.89312	0.21376
31	C	4.00000	1.97739	1.97739	0.04522
32	C	4.00000	1.97976	1.97976	0.04047
33	C	4.00000	2.01300	2.01300	-0.02600
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>2.22756</b>	<b>2.22756</b>	<b>-0.45512</b>
35	C	4.00000	1.87967	1.87967	0.24067
36	C	4.00000	1.98582	1.98582	0.02836
37	C	4.00000	1.98205	1.98205	0.03590
38	C	4.00000	1.98917	1.98917	0.02166
39	C	4.00000	2.22396	2.22396	-0.44793
40	I	7.00000	3.42898	3.42898	0.14204
41	I	7.00000	3.42841	3.42841	0.14318
42	I	7.00000	3.42893	3.42893	0.14213
43	I	7.00000	3.42860	3.42860	0.14280
44	I	7.00000	3.42815	3.42815	0.14371
45	I	7.00000	3.42884	3.42884	0.14233
46	I	7.00000	3.43063	3.43063	0.13874
47	I	7.00000	3.42845	3.42845	0.14310
48	C	4.00000	1.92456	1.92456	0.15088
-----					
total charge		216.00000	108.00000	108.00000	0.00000
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**b. OOH**

	iatm	typnm	znuc	rho(u)	rho(d)	popul
-----						
1	C	4.00000	2.38364	2.05893	-0.44257	
2	C	4.00000	2.07083	1.97675	-0.04758	



3	C	4.00000	1.99686	1.96280	0.04035
4	C	4.00000	1.99432	1.97775	0.02794
5	C	4.00000	1.93562	1.92169	0.14269
6	C	4.00000	2.39199	2.07322	-0.46521
7	C	4.00000	2.02618	1.93297	0.04085
8	C	4.00000	1.95359	1.98599	0.06042
9	C	4.00000	1.98184	1.96556	0.05260
10	C	4.00000	1.92951	1.91523	0.15525
11	C	4.00000	2.38143	2.05981	-0.44124
12	C	4.00000	2.06356	1.97150	-0.03506
13	C	4.00000	2.00138	1.96678	0.03183
14	C	4.00000	2.00314	1.98676	0.01010
15	C	4.00000	1.94103	1.92623	0.13274
16	C	4.00000	2.39370	2.06989	-0.46359
17	C	4.00000	2.02838	1.93599	0.03563
18	C	4.00000	1.92333	1.88943	0.18724
19	C	4.00000	1.94020	1.91944	0.14036
20	C	4.00000	1.91154	1.89752	0.19094
21	C	4.00000	1.83335	1.95784	0.20880
22	C	4.00000	1.94109	1.99916	0.05975
23	C	4.00000	1.95988	1.98804	0.05207
24	C	4.00000	1.97380	1.98833	0.03787
25	C	4.00000	2.19515	2.23380	-0.42895
26	C	4.00000	1.81857	1.94293	0.23850
27	C	4.00000	1.98546	2.04041	-0.02587
28	C	4.00000	1.95690	1.97070	0.07240
29	C	4.00000	2.22287	2.25231	-0.47518
30	C	4.00000	1.83207	1.95775	0.21018
31	C	4.00000	1.94951	2.00534	0.04514
32	C	4.00000	1.96244	1.99092	0.04664
33	C	4.00000	2.00240	2.02730	-0.02970
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>2.05767</b>	<b>2.05905</b>	<b>-0.11672</b>
35	C	4.00000	1.81912	1.94492	0.23596

36	C	4.00000	1.98180	2.03860	-0.02040
37	C	4.00000	1.96291	1.98759	0.04950
38	C	4.00000	1.98694	2.01261	0.00045
39	C	4.00000	2.22633	2.25202	-0.47834
40	I	7.00000	3.47653	3.47670	0.04678
41	I	7.00000	3.42664	3.42869	0.14467
42	I	7.00000	3.43061	3.43303	0.13636
43	I	7.00000	3.44092	3.41689	0.14218
44	I	7.00000	3.44161	3.41815	0.14023
45	I	7.00000	3.44075	3.41702	0.14223
46	I	7.00000	3.44135	3.41764	0.14101
47	I	7.00000	3.42984	3.43159	0.13858
48	C	4.00000	1.94089	1.90669	0.15242
49	O	6.00000	3.12155	3.12093	-0.24248
50	O	6.00000	3.18654	3.18644	-0.37299
51	H	1.00000	0.30239	0.30239	0.39521

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total charge	229.00000	115.00000	114.00000	0.00000
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**c. O**

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	iatm	typnm	znuc	rho(u)	rho(d)	popul
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1	C	4.00000	2.22551	2.22551	-0.45102
2	C	4.00000	2.01303	2.01303	-0.02606
3	C	4.00000	1.97741	1.97741	0.04518
4	C	4.00000	1.97893	1.97893	0.04215
5	C	4.00000	1.92986	1.92986	0.14028
6	C	4.00000	2.23130	2.23130	-0.46259
7	C	4.00000	1.99230	1.99230	0.01540
8	C	4.00000	1.98107	1.98107	0.03785
9	C	4.00000	1.97029	1.97029	0.05942
10	C	4.00000	1.91742	1.91742	0.16516

11	C	4.00000	2.22712	2.22712	-0.45425
12	C	4.00000	2.02333	2.02333	-0.04665
13	C	4.00000	1.98190	1.98190	0.03621
14	C	4.00000	2.01175	2.01175	-0.02351
15	C	4.00000	1.96811	1.96811	0.06377
16	C	4.00000	2.23088	2.23088	-0.46177
17	C	4.00000	1.98026	1.98026	0.03947
18	C	4.00000	1.92424	1.92424	0.15151
19	C	4.00000	2.02956	2.02956	-0.05912
20	C	4.00000	1.92925	1.92925	0.14149
21	C	4.00000	1.89170	1.89170	0.21660
22	C	4.00000	1.97880	1.97880	0.04240
23	C	4.00000	1.96054	1.96054	0.07891
24	C	4.00000	1.99077	1.99077	0.01845
25	C	4.00000	2.21176	2.21176	-0.42351
26	C	4.00000	1.88160	1.88160	0.23681
27	C	4.00000	1.98068	1.98068	0.03863
28	C	4.00000	1.94378	1.94378	0.11244
29	C	4.00000	2.19210	2.19210	-0.38420
30	C	4.00000	1.89131	1.89131	0.21737
31	C	4.00000	1.97456	1.97456	0.05089
32	C	4.00000	1.99133	1.99133	0.01735
33	C	4.00000	1.92854	1.92854	0.14293
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>2.02414</b>	<b>2.02414</b>	<b>-0.04827</b>
35	C	4.00000	1.88175	1.88175	0.23650
36	C	4.00000	2.00955	2.00955	-0.01909
37	C	4.00000	1.96038	1.96038	0.07924
38	C	4.00000	1.96029	1.96029	0.07942
39	C	4.00000	2.22750	2.22750	-0.45500
40	I	7.00000	3.45800	3.45800	0.08401
41	I	7.00000	3.42103	3.42103	0.15795
42	I	7.00000	3.42350	3.42350	0.15301
43	I	7.00000	3.42714	3.42714	0.14571

44	I	7.00000	3.42845	3.42845	0.14311
45	I	7.00000	3.42741	3.42741	0.14518
46	I	7.00000	3.42841	3.42841	0.14317
47	I	7.00000	3.42580	3.42580	0.14840
48	C	4.00000	1.94930	1.94930	0.10140
49	O	6.00000	3.20637	3.20637	-0.41275

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total charge	222.00000	111.00000	111.00000	0.00000
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#### d. OH

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	iatm	typnm	znuc	rho(u)	rho(d)	popul
	1	C	4.00000	2.38363	2.05814	-0.44177
	2	C	4.00000	2.07745	1.98225	-0.05970
	3	C	4.00000	1.99818	1.96366	0.03816
	4	C	4.00000	1.98178	1.96533	0.05289
	5	C	4.00000	1.93158	1.91774	0.15068
	6	C	4.00000	2.38883	2.06932	-0.45815
	7	C	4.00000	2.01975	1.92598	0.05427
	8	C	4.00000	1.95319	1.98621	0.06060
	9	C	4.00000	1.99490	1.97860	0.02650
	10	C	4.00000	1.92184	1.90788	0.17028
	11	C	4.00000	2.38248	2.05885	-0.44133
	12	C	4.00000	2.07138	1.97829	-0.04967
	13	C	4.00000	2.00779	1.97242	0.01978
	14	C	4.00000	1.99640	1.97994	0.02366
	15	C	4.00000	1.93524	1.92054	0.14421
	16	C	4.00000	2.39130	2.06644	-0.45774
	17	C	4.00000	2.02207	1.92912	0.04881
	18	C	4.00000	1.93652	1.90243	0.16104
	19	C	4.00000	1.96781	1.94707	0.08512

20	C	4.00000	1.93983	1.92580	0.13437
21	C	4.00000	1.83485	1.96057	0.20459
22	C	4.00000	1.94201	2.00089	0.05710
23	C	4.00000	1.95822	1.98704	0.05474
24	C	4.00000	1.98783	2.00224	0.00993
25	C	4.00000	2.19700	2.23571	-0.43272
26	C	4.00000	1.81750	1.94290	0.23961
27	C	4.00000	1.97542	2.03116	-0.00657
28	C	4.00000	1.95336	1.96756	0.07908
29	C	4.00000	2.22657	2.25330	-0.47987
30	C	4.00000	1.83223	1.95951	0.20826
31	C	4.00000	1.94817	2.00503	0.04681
32	C	4.00000	1.95523	1.98408	0.06069
33	C	4.00000	1.99857	2.02421	-0.02278
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>2.05532</b>	<b>2.05676</b>	<b>-0.11208</b>
35	C	4.00000	1.81821	1.94477	0.23702
36	C	4.00000	1.98263	2.04062	-0.02325
37	C	4.00000	1.95049	1.97516	0.07435
38	C	4.00000	1.98469	2.01036	0.00495
39	C	4.00000	2.22457	2.25014	-0.47471
40	I	7.00000	3.47713	3.47741	0.04546
41	I	7.00000	3.42864	3.43045	0.14091
42	I	7.00000	3.43180	3.43439	0.13380
43	I	7.00000	3.44133	3.41775	0.14092
44	I	7.00000	3.44159	3.41798	0.14043
45	I	7.00000	3.44113	3.41775	0.14112
46	I	7.00000	3.44151	3.41767	0.14082
47	I	7.00000	3.42748	3.42910	0.14342
48	C	4.00000	1.95690	1.92236	0.12074
49	O	6.00000	3.27314	3.27263	-0.54578
50	H	1.00000	0.29451	0.29449	0.41100

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total charge	223.00000	112.00000	111.00000	0.00000
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**e. HOH formation Transition State**

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iatm	typnm	znuc	rho(u)	rho(d)	popul
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1	C	4.00000	2.21982	2.21982	-0.43965
2	C	4.00000	2.02012	2.02012	-0.04023
3	C	4.00000	2.00303	2.00303	-0.00607
4	C	4.00000	1.99436	1.99436	0.01129
5	C	4.00000	1.92969	1.92969	0.14062
6	C	4.00000	2.23858	2.23858	-0.47717
7	C	4.00000	1.95854	1.95854	0.08291
8	C	4.00000	1.97809	1.97809	0.04383
9	C	4.00000	1.96423	1.96423	0.07153
10	C	4.00000	1.91339	1.91339	0.17321
11	C	4.00000	2.22560	2.22560	-0.45120
12	C	4.00000	2.02251	2.02251	-0.04502
13	C	4.00000	2.00299	2.00299	-0.00597
14	C	4.00000	2.02406	2.02406	-0.04813
15	C	4.00000	1.96933	1.96933	0.06133
16	C	4.00000	2.23664	2.23664	-0.47327
17	C	4.00000	2.00365	2.00365	-0.00729
18	C	4.00000	1.95095	1.95095	0.09810
19	C	4.00000	1.99806	1.99806	0.00389
20	C	4.00000	1.92827	1.92827	0.14346
21	C	4.00000	1.89119	1.89119	0.21762
22	C	4.00000	1.99965	1.99965	0.00070
23	C	4.00000	2.01038	2.01038	-0.02077
24	C	4.00000	1.99782	1.99782	0.00436
25	C	4.00000	2.19426	2.19426	-0.38853
26	C	4.00000	1.87946	1.87946	0.24109
27	C	4.00000	2.00327	2.00327	-0.00655

28	C	4.00000	1.92497	1.92497	0.15006
29	C	4.00000	2.26351	2.26351	-0.52702
30	C	4.00000	1.88722	1.88722	0.22555
31	C	4.00000	1.95852	1.95852	0.08297
32	C	4.00000	1.95725	1.95725	0.08550
33	C	4.00000	1.96588	1.96588	0.06824
<b>34</b>	<b>C</b>	<b>4.00000</b>	<b>2.07568</b>	<b>2.07568</b>	<b>-0.15136</b>
35	C	4.00000	1.87513	1.87513	0.24973
36	C	4.00000	1.96451	1.96451	0.07097
37	C	4.00000	1.94003	1.94003	0.11994
38	C	4.00000	1.95161	1.95161	0.09678
39	C	4.00000	2.24295	2.24295	-0.48589
40	I	7.00000	3.46602	3.46602	0.06796
41	I	7.00000	3.54542	3.54542	-0.09085
42	I	7.00000	3.42180	3.42180	0.15640
43	I	7.00000	3.42889	3.42889	0.14221
44	I	7.00000	3.42743	3.42743	0.14515
45	I	7.00000	3.43234	3.43234	0.13532
46	I	7.00000	3.42366	3.42366	0.15268
47	I	7.00000	3.40825	3.40825	0.18350
48	C	4.00000	1.92670	1.92670	0.14659
49	O	6.00000	3.31087	3.31087	-0.62174
50	H	1.00000	0.29170	0.29170	0.41660
51	H	1.00000	0.28051	0.28051	0.43899
52	O	6.00000	3.41235	3.41235	-0.82470
53	H	1.00000	0.30043	0.30043	0.39914
54	H	1.00000	0.35841	0.35841	0.28318
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total charge		232.00000	116.00000	116.00000	0.00000
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